



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 09:55 pm GMT

PDB ID : 7PNB
EMDB ID : EMD-13546
Title : Sulfolobus acidocaldarius 0406 filament.
Authors : Isupov, M.N.; Gaines, M.; Daum, B.
Deposited on : 2021-09-06
Resolution : 3.46 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

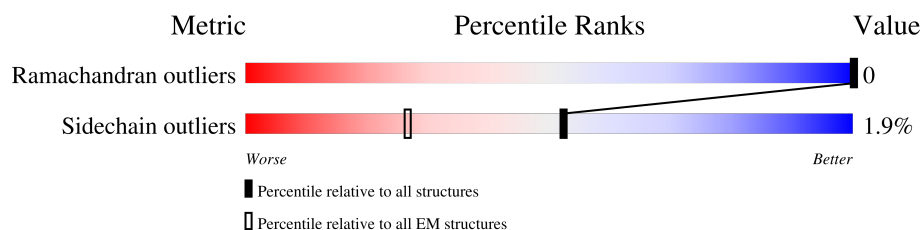
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY







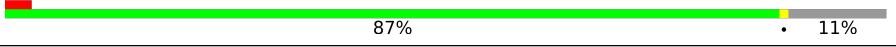


The reported resolution of this entry is 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	
1	B	206	
1	C	206	
1	D	206	
1	E	206	
1	F	206	
1	G	206	
1	H	206	
1	I	206	

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Mol	Chain	Length	Quality of chain
2	0	6	
2	1	6	
2	J	6	
2	L	6	
2	M	6	
2	N	6	
2	O	6	
2	Q	6	
2	R	6	
2	S	6	
2	T	6	
2	V	6	
2	W	6	
2	X	6	
2	Y	6	
2	a	6	
2	b	6	
2	c	6	
2	d	6	
2	f	6	
2	g	6	
2	h	6	
2	i	6	
2	k	6	
2	l	6	

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Mol	Chain	Length	Quality of chain
2	m	6	<div>83%</div> <div> <div></div> <div>33%</div> <div>67%</div> </div>
2	n	6	<div>33%</div> <div> <div></div> <div>50%</div> <div>50%</div> </div>
2	p	6	<div>67%</div> <div> <div></div> <div>100%</div> </div>
2	q	6	<div>50%</div> <div> <div></div> <div>17%</div> <div>83%</div> </div>
2	r	6	<div>83%</div> <div> <div></div> <div>33%</div> <div>67%</div> </div>
2	s	6	<div>50%</div> <div> <div></div> <div>50%</div> <div>50%</div> </div>
2	u	6	<div>67%</div> <div> <div></div> <div>17%</div> <div>83%</div> </div>
2	v	6	<div>50%</div> <div> <div></div> <div>17%</div> <div>83%</div> </div>
2	w	6	<div>83%</div> <div> <div></div> <div>33%</div> <div>67%</div> </div>
2	x	6	<div>100%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div>
2	z	6	<div>100%</div> <div> <div></div> <div>100%</div> </div>
3	K	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	P	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	U	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	Z	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	e	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	j	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	o	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	t	4	<div>75%</div> <div> <div></div> <div>100%</div> </div>
3	y	4	<div>100%</div> <div> <div></div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15714 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called *Sulfolobus acidocaldarius* 0406 filament..

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	B	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	C	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	D	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	E	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	F	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	G	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	H	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		
1	I	183	Total	C	N	O	S	0	0
			1393	903	219	267	4		

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
2	L	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
2	M	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
2	N	6	Total	C	N	O	S	0	0
			75	40	2	32	1		
2	O	6	Total	C	N	O	S	0	0
			75	40	2	32	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	R	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	S	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	T	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	V	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	W	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	X	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	Y	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	a	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	b	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	c	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	d	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	f	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	g	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	h	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	i	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	k	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	l	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	m	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	n	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	p	6	Total 75	C 40	N 2	O 32	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	q	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	r	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	s	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	u	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	v	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	w	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	x	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	z	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	0	6	Total 75	C 40	N 2	O 32	S 1	0	0
2	1	6	Total 75	C 40	N 2	O 32	S 1	0	0

- Molecule 3 is an oligosaccharide called 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	P	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	U	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	Z	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	e	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	j	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	o	4	Total 53	C 28	N 2	O 22	S 1	0	0
3	t	4	Total 53	C 28	N 2	O 22	S 1	0	0

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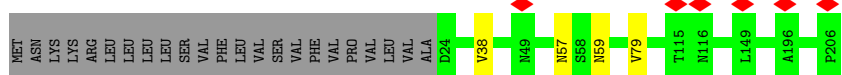
Mol	Chain	Residues	Atoms					AltConf	Trace
3	y	4	Total	C	N	O	S	0	0
			53	28	2	22	1		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

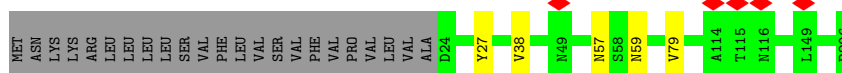
- Molecule 1: *Sulfolobus acidocaldarius* 0406 filament.

Chain A: 




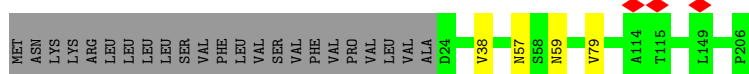
- Molecule 1: *Sulfolobus acidocaldarius* 0406 filament.

Chain B: 




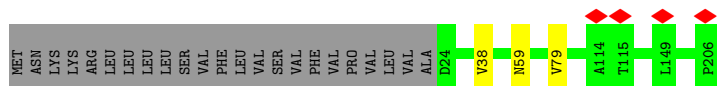
- Molecule 1: *Sulfolobus acidocaldarius* 0406 filament.

Chain C: 




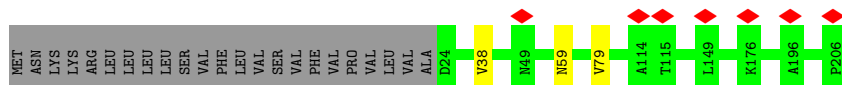
- Molecule 1: *Sulfolobus acidocaldarius* 0406 filament.

Chain D: 




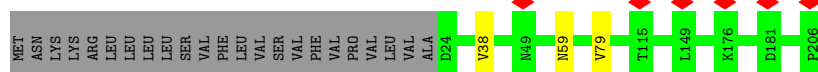
- Molecule 1: *Sulfolobus acidocaldarius* 0406 filament.

Chain E: 



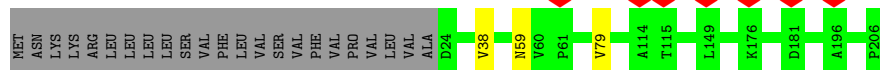
- Molecule 1: *Sulfolobus acidocaldarius* 0406 filament.

Chain F:  87% 11%



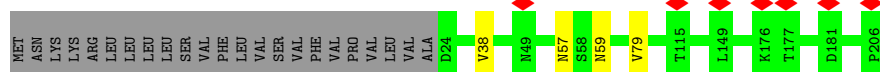
- Molecule 1: Sulfolobus acidocaldarius 0406 filament.

Chain G:  87% 11%




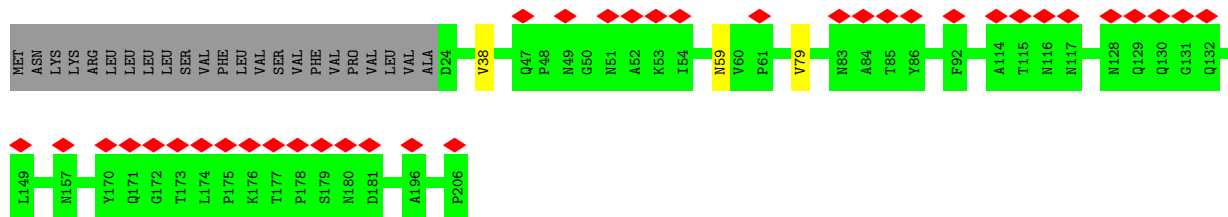
- Molecule 1: Sulfolobus acidocaldarius 0406 filament.

Chain H:  87% 11%



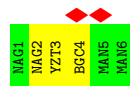
- Molecule 1: Sulfolobus acidocaldarius 0406 filament.

Chain I:  18% 87% 11%



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 50% 50%

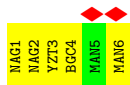


- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  17% 100%



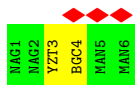
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



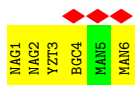
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



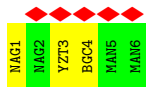
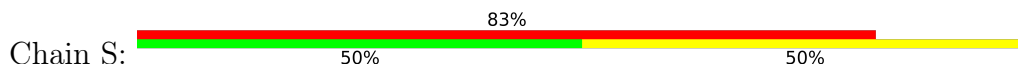
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



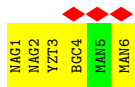
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



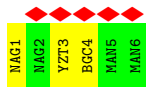
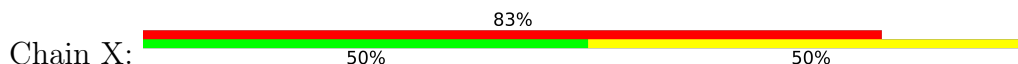
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



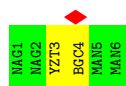
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-m

annopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 



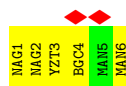
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 



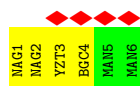
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

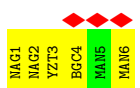


- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



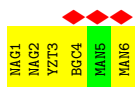
● Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



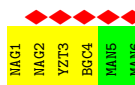
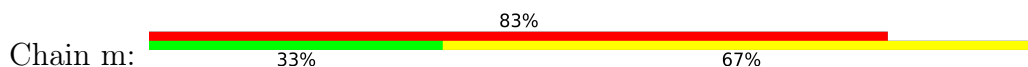
● Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



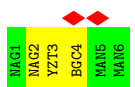
● Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



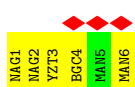
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



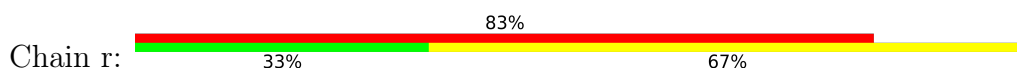
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



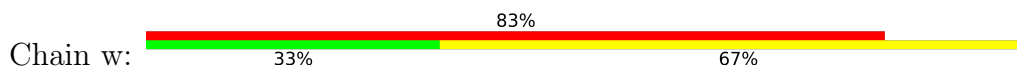
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

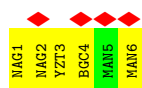




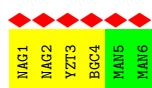
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



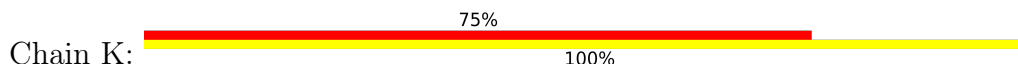
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



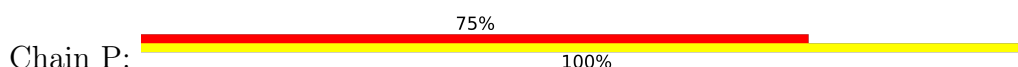
- Molecule 2: beta-D-glucopyranose-(1-4)-6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)][alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

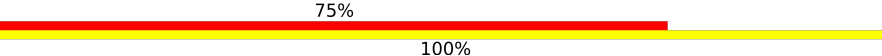


- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 




- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

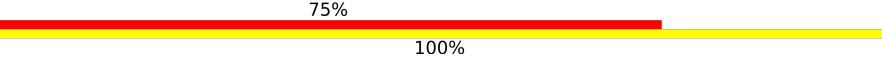


- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 




- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 




- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t: 



- Molecule 3: 6-deoxy-6-sulfo-beta-D-glucopyranose-(1-3)-[alpha-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  100%

100%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-103.234°, rise=31.649 Å, axial sym=C1	Depositor
Number of segments used	188620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	42.33	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.567	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1638	Depositor
Map size (Å)	402.04803, 402.04803, 402.04803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NAG, MAN, YZT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/1433	0.74	1/1969 (0.1%)
1	B	0.42	0/1433	0.74	2/1969 (0.1%)
1	C	0.43	0/1433	0.74	1/1969 (0.1%)
1	D	0.42	0/1433	0.74	0/1969
1	E	0.42	0/1433	0.74	0/1969
1	F	0.42	0/1433	0.74	0/1969
1	G	0.42	0/1433	0.74	0/1969
1	H	0.42	0/1433	0.74	1/1969 (0.1%)
1	I	0.39	0/1433	0.71	0/1969
All	All	0.42	0/12897	0.74	5/17721 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	57	ASN	CB-CA-C	-5.07	100.26	110.40
1	A	57	ASN	CB-CA-C	-5.07	100.26	110.40
1	C	57	ASN	CB-CA-C	-5.04	100.32	110.40
1	H	57	ASN	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	B	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	C	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	D	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	E	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	F	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	G	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	H	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
1	I	181/206 (88%)	171 (94%)	10 (6%)	0	100	100
All	All	1629/1854 (88%)	1539 (94%)	90 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	B	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	C	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	D	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	E	156/178 (88%)	153 (98%)	3 (2%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	G	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	H	156/178 (88%)	153 (98%)	3 (2%)	52	74
1	I	156/178 (88%)	153 (98%)	3 (2%)	52	74
All	All	1404/1602 (88%)	1377 (98%)	27 (2%)	52	74

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	59	ASN
1	A	79	VAL
1	B	38	VAL
1	B	59	ASN
1	B	79	VAL
1	C	38	VAL
1	C	59	ASN
1	C	79	VAL
1	D	38	VAL
1	D	59	ASN
1	D	79	VAL
1	E	38	VAL
1	E	59	ASN
1	E	79	VAL
1	F	38	VAL
1	F	59	ASN
1	F	79	VAL
1	G	38	VAL
1	G	59	ASN
1	G	79	VAL
1	H	38	VAL
1	H	59	ASN
1	H	79	VAL
1	I	38	VAL
1	I	59	ASN
1	I	79	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	B	37	ASN
1	B	129	GLN
1	C	37	ASN
1	C	129	GLN
1	D	37	ASN
1	D	129	GLN
1	E	37	ASN
1	E	129	GLN
1	F	37	ASN
1	F	129	GLN
1	G	37	ASN
1	G	129	GLN
1	H	37	ASN
1	H	129	GLN
1	I	129	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

252 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	0	1	1,2	14,14,15	0.94	0	17,19,21	1.45	3 (17%)
2	NAG	0	2	2	14,14,15	0.46	0	17,19,21	1.90	5 (29%)
2	YZT	0	3	2	13,14,15	1.07	1 (7%)	18,21,23	1.85	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	0	4	2	11,11,12	0.28	0	15,15,17	1.21	2 (13%)
2	MAN	0	5	2	11,11,12	0.47	0	15,15,17	0.69	0
2	MAN	0	6	2	11,11,12	0.47	0	15,15,17	0.94	1 (6%)
2	NAG	1	1	1,2	14,14,15	0.62	0	17,19,21	1.03	2 (11%)
2	NAG	1	2	2	14,14,15	0.47	0	17,19,21	0.90	1 (5%)
2	YZT	1	3	2	13,14,15	1.15	1 (7%)	18,21,23	1.39	2 (11%)
2	BGC	1	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.35	3 (20%)
2	MAN	1	5	2	11,11,12	0.48	0	15,15,17	0.96	0
2	MAN	1	6	2	11,11,12	0.48	0	15,15,17	1.02	0
2	NAG	J	1	1,2	14,14,15	0.40	0	17,19,21	0.82	0
2	NAG	J	2	2	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
2	YZT	J	3	2	13,14,15	1.23	1 (7%)	18,21,23	1.07	1 (5%)
2	BGC	J	4	2	11,11,12	0.25	0	15,15,17	1.06	1 (6%)
2	MAN	J	5	2	11,11,12	0.41	0	15,15,17	0.72	0
2	MAN	J	6	2	11,11,12	0.42	0	15,15,17	0.82	0
3	NAG	K	1	3,1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
3	NAG	K	2	3	14,14,15	0.47	0	17,19,21	1.75	5 (29%)
3	YZT	K	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	3 (16%)
3	MAN	K	4	3	11,11,12	0.82	0	15,15,17	2.71	5 (33%)
2	NAG	L	1	1,2	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
2	NAG	L	2	2	14,14,15	0.57	0	17,19,21	1.09	1 (5%)
2	YZT	L	3	2	13,14,15	1.32	2 (15%)	18,21,23	1.59	3 (16%)
2	BGC	L	4	2	11,11,12	0.97	1 (9%)	15,15,17	2.06	6 (40%)
2	MAN	L	5	2	11,11,12	0.49	0	15,15,17	1.16	2 (13%)
2	MAN	L	6	2	11,11,12	0.53	0	15,15,17	1.13	1 (6%)
2	NAG	M	1	1,2	14,14,15	1.25	2 (14%)	17,19,21	1.72	4 (23%)
2	NAG	M	2	2	14,14,15	0.56	0	17,19,21	1.98	5 (29%)
2	YZT	M	3	2	13,14,15	1.18	1 (7%)	18,21,23	1.96	3 (16%)
2	BGC	M	4	2	11,11,12	0.32	0	15,15,17	1.30	2 (13%)
2	MAN	M	5	2	11,11,12	0.49	0	15,15,17	0.71	0
2	MAN	M	6	2	11,11,12	0.51	0	15,15,17	0.96	1 (6%)
2	NAG	N	1	1,2	14,14,15	0.68	0	17,19,21	1.34	3 (17%)
2	NAG	N	2	2	14,14,15	0.46	0	17,19,21	0.91	0
2	YZT	N	3	2	13,14,15	1.14	1 (7%)	18,21,23	1.36	2 (11%)
2	BGC	N	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.34	3 (20%)
2	MAN	N	5	2	11,11,12	0.49	0	15,15,17	0.97	0
2	MAN	N	6	2	11,11,12	0.47	0	15,15,17	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	O	1	1,2	14,14,15	0.34	0	17,19,21	0.84	0
2	NAG	O	2	2	14,14,15	0.47	0	17,19,21	0.79	0
2	YZT	O	3	2	13,14,15	1.27	1 (7%)	18,21,23	1.13	1 (5%)
2	BGC	O	4	2	11,11,12	0.23	0	15,15,17	1.09	2 (13%)
2	MAN	O	5	2	11,11,12	0.42	0	15,15,17	0.72	0
2	MAN	O	6	2	11,11,12	0.40	0	15,15,17	0.82	0
3	NAG	P	1	3,1	14,14,15	0.67	0	17,19,21	1.05	1 (5%)
3	NAG	P	2	3	14,14,15	0.47	0	17,19,21	1.75	5 (29%)
3	YZT	P	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	3 (16%)
3	MAN	P	4	3	11,11,12	0.84	0	15,15,17	2.71	5 (33%)
2	NAG	Q	1	1,2	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
2	NAG	Q	2	2	14,14,15	0.60	0	17,19,21	1.09	1 (5%)
2	YZT	Q	3	2	13,14,15	1.31	2 (15%)	18,21,23	1.58	3 (16%)
2	BGC	Q	4	2	11,11,12	0.97	1 (9%)	15,15,17	2.05	7 (46%)
2	MAN	Q	5	2	11,11,12	0.51	0	15,15,17	1.17	2 (13%)
2	MAN	Q	6	2	11,11,12	0.65	0	15,15,17	1.15	2 (13%)
2	NAG	R	1	1,2	14,14,15	1.17	2 (14%)	17,19,21	1.59	4 (23%)
2	NAG	R	2	2	14,14,15	0.57	0	17,19,21	1.94	5 (29%)
2	YZT	R	3	2	13,14,15	1.17	1 (7%)	18,21,23	1.84	3 (16%)
2	BGC	R	4	2	11,11,12	0.30	0	15,15,17	1.25	2 (13%)
2	MAN	R	5	2	11,11,12	0.49	0	15,15,17	0.69	0
2	MAN	R	6	2	11,11,12	0.54	0	15,15,17	0.96	1 (6%)
2	NAG	S	1	1,2	14,14,15	0.73	0	17,19,21	1.20	3 (17%)
2	NAG	S	2	2	14,14,15	0.48	0	17,19,21	0.87	0
2	YZT	S	3	2	13,14,15	1.15	1 (7%)	18,21,23	1.41	2 (11%)
2	BGC	S	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.35	3 (20%)
2	MAN	S	5	2	11,11,12	0.51	0	15,15,17	0.96	0
2	MAN	S	6	2	11,11,12	0.48	0	15,15,17	1.01	0
2	NAG	T	1	1,2	14,14,15	0.41	0	17,19,21	0.89	0
2	NAG	T	2	2	14,14,15	0.46	0	17,19,21	0.75	0
2	YZT	T	3	2	13,14,15	1.24	1 (7%)	18,21,23	1.17	1 (5%)
2	BGC	T	4	2	11,11,12	0.25	0	15,15,17	1.11	2 (13%)
2	MAN	T	5	2	11,11,12	0.37	0	15,15,17	0.70	0
2	MAN	T	6	2	11,11,12	0.38	0	15,15,17	0.86	0
3	NAG	U	1	3,1	14,14,15	0.71	0	17,19,21	1.08	1 (5%)
3	NAG	U	2	3	14,14,15	0.49	0	17,19,21	1.77	5 (29%)
3	YZT	U	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.37	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	U	4	3	11,11,12	0.83	0	15,15,17	2.71	5 (33%)
2	NAG	V	1	1,2	14,14,15	0.92	0	17,19,21	1.06	1 (5%)
2	NAG	V	2	2	14,14,15	0.56	0	17,19,21	1.08	1 (5%)
2	YZT	V	3	2	13,14,15	1.32	2 (15%)	18,21,23	1.59	3 (16%)
2	BGC	V	4	2	11,11,12	0.96	1 (9%)	15,15,17	2.05	6 (40%)
2	MAN	V	5	2	11,11,12	0.45	0	15,15,17	1.14	2 (13%)
2	MAN	V	6	2	11,11,12	0.59	0	15,15,17	1.07	1 (6%)
2	NAG	W	1	1,2	14,14,15	1.15	2 (14%)	17,19,21	1.62	4 (23%)
2	NAG	W	2	2	14,14,15	0.58	0	17,19,21	1.91	5 (29%)
2	YZT	W	3	2	13,14,15	1.29	1 (7%)	18,21,23	1.96	2 (11%)
2	BGC	W	4	2	11,11,12	0.30	0	15,15,17	1.26	2 (13%)
2	MAN	W	5	2	11,11,12	0.49	0	15,15,17	0.70	0
2	MAN	W	6	2	11,11,12	0.57	0	15,15,17	0.99	1 (6%)
2	NAG	X	1	1,2	14,14,15	0.76	0	17,19,21	1.17	2 (11%)
2	NAG	X	2	2	14,14,15	0.47	0	17,19,21	0.88	0
2	YZT	X	3	2	13,14,15	1.12	1 (7%)	18,21,23	1.39	2 (11%)
2	BGC	X	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.34	3 (20%)
2	MAN	X	5	2	11,11,12	0.50	0	15,15,17	0.97	0
2	MAN	X	6	2	11,11,12	0.49	0	15,15,17	1.00	0
2	NAG	Y	1	1,2	14,14,15	0.42	0	17,19,21	0.78	0
2	NAG	Y	2	2	14,14,15	0.49	0	17,19,21	0.79	0
2	YZT	Y	3	2	13,14,15	1.28	1 (7%)	18,21,23	1.16	1 (5%)
2	BGC	Y	4	2	11,11,12	0.26	0	15,15,17	1.08	1 (6%)
2	MAN	Y	5	2	11,11,12	0.39	0	15,15,17	0.71	0
2	MAN	Y	6	2	11,11,12	0.38	0	15,15,17	0.85	0
3	NAG	Z	1	3,1	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
3	NAG	Z	2	3	14,14,15	0.50	0	17,19,21	1.76	5 (29%)
3	YZT	Z	3	3	13,14,15	1.06	1 (7%)	18,21,23	1.36	3 (16%)
3	MAN	Z	4	3	11,11,12	0.84	0	15,15,17	2.70	5 (33%)
2	NAG	a	1	1,2	14,14,15	0.80	0	17,19,21	0.98	1 (5%)
2	NAG	a	2	2	14,14,15	0.51	0	17,19,21	1.04	1 (5%)
2	YZT	a	3	2	13,14,15	1.33	2 (15%)	18,21,23	1.58	3 (16%)
2	BGC	a	4	2	11,11,12	0.96	1 (9%)	15,15,17	2.06	7 (46%)
2	MAN	a	5	2	11,11,12	0.48	0	15,15,17	1.13	2 (13%)
2	MAN	a	6	2	11,11,12	0.55	0	15,15,17	1.11	1 (6%)
2	NAG	b	1	1,2	14,14,15	1.11	2 (14%)	17,19,21	1.60	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	b	2	2	14,14,15	0.55	0	17,19,21	1.92	5 (29%)
2	YZT	b	3	2	13,14,15	1.24	1 (7%)	18,21,23	1.96	2 (11%)
2	BGC	b	4	2	11,11,12	0.31	0	15,15,17	1.27	2 (13%)
2	MAN	b	5	2	11,11,12	0.50	0	15,15,17	0.69	0
2	MAN	b	6	2	11,11,12	0.53	0	15,15,17	0.97	1 (6%)
2	NAG	c	1	1,2	14,14,15	0.72	0	17,19,21	1.24	2 (11%)
2	NAG	c	2	2	14,14,15	0.46	0	17,19,21	0.90	1 (5%)
2	YZT	c	3	2	13,14,15	1.13	1 (7%)	18,21,23	1.36	2 (11%)
2	BGC	c	4	2	11,11,12	0.84	1 (9%)	15,15,17	1.34	3 (20%)
2	MAN	c	5	2	11,11,12	0.49	0	15,15,17	0.96	0
2	MAN	c	6	2	11,11,12	0.47	0	15,15,17	1.01	0
2	NAG	d	1	1,2	14,14,15	0.45	0	17,19,21	0.85	0
2	NAG	d	2	2	14,14,15	0.56	0	17,19,21	0.82	1 (5%)
2	YZT	d	3	2	13,14,15	1.41	1 (7%)	18,21,23	1.10	2 (11%)
2	BGC	d	4	2	11,11,12	0.24	0	15,15,17	1.12	2 (13%)
2	MAN	d	5	2	11,11,12	0.41	0	15,15,17	0.73	0
2	MAN	d	6	2	11,11,12	0.39	0	15,15,17	0.82	0
3	NAG	e	1	3,1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
3	NAG	e	2	3	14,14,15	0.48	0	17,19,21	1.76	5 (29%)
3	YZT	e	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	3 (16%)
3	MAN	e	4	3	11,11,12	0.84	0	15,15,17	2.70	5 (33%)
2	NAG	f	1	1,2	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
2	NAG	f	2	2	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
2	YZT	f	3	2	13,14,15	1.30	1 (7%)	18,21,23	1.66	3 (16%)
2	BGC	f	4	2	11,11,12	0.99	1 (9%)	15,15,17	2.07	7 (46%)
2	MAN	f	5	2	11,11,12	0.48	0	15,15,17	1.11	2 (13%)
2	MAN	f	6	2	11,11,12	0.53	0	15,15,17	1.11	1 (6%)
2	NAG	g	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	1.57	4 (23%)
2	NAG	g	2	2	14,14,15	0.48	0	17,19,21	1.88	5 (29%)
2	YZT	g	3	2	13,14,15	1.16	1 (7%)	18,21,23	1.91	3 (16%)
2	BGC	g	4	2	11,11,12	0.34	0	15,15,17	1.26	2 (13%)
2	MAN	g	5	2	11,11,12	0.51	0	15,15,17	0.71	0
2	MAN	g	6	2	11,11,12	0.51	0	15,15,17	0.96	1 (6%)
2	NAG	h	1	1,2	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
2	NAG	h	2	2	14,14,15	0.45	0	17,19,21	0.91	0
2	YZT	h	3	2	13,14,15	1.13	1 (7%)	18,21,23	1.35	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	h	4	2	11,11,12	0.85	1 (9%)	15,15,17	1.34	3 (20%)
2	MAN	h	5	2	11,11,12	0.48	0	15,15,17	0.97	0
2	MAN	h	6	2	11,11,12	0.48	0	15,15,17	1.01	0
2	NAG	i	1	1,2	14,14,15	0.39	0	17,19,21	0.84	0
2	NAG	i	2	2	14,14,15	0.54	0	17,19,21	0.81	0
2	YZT	i	3	2	13,14,15	1.27	1 (7%)	18,21,23	1.10	1 (5%)
2	BGC	i	4	2	11,11,12	0.26	0	15,15,17	1.11	2 (13%)
2	MAN	i	5	2	11,11,12	0.39	0	15,15,17	0.73	0
2	MAN	i	6	2	11,11,12	0.40	0	15,15,17	0.80	0
3	NAG	j	1	3,1	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
3	NAG	j	2	3	14,14,15	0.49	0	17,19,21	1.77	5 (29%)
3	YZT	j	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	3 (16%)
3	MAN	j	4	3	11,11,12	0.82	0	15,15,17	2.71	5 (33%)
2	NAG	k	1	1,2	14,14,15	0.83	0	17,19,21	1.01	1 (5%)
2	NAG	k	2	2	14,14,15	0.57	0	17,19,21	1.07	2 (11%)
2	YZT	k	3	2	13,14,15	1.41	2 (15%)	18,21,23	1.61	3 (16%)
2	BGC	k	4	2	11,11,12	0.97	1 (9%)	15,15,17	2.07	6 (40%)
2	MAN	k	5	2	11,11,12	0.47	0	15,15,17	1.18	2 (13%)
2	MAN	k	6	2	11,11,12	0.50	0	15,15,17	1.13	1 (6%)
2	NAG	l	1	1,2	14,14,15	1.19	1 (7%)	17,19,21	1.72	4 (23%)
2	NAG	l	2	2	14,14,15	0.52	0	17,19,21	1.88	5 (29%)
2	YZT	l	3	2	13,14,15	1.23	1 (7%)	18,21,23	2.00	3 (16%)
2	BGC	l	4	2	11,11,12	0.33	0	15,15,17	1.24	2 (13%)
2	MAN	l	5	2	11,11,12	0.53	0	15,15,17	0.72	0
2	MAN	l	6	2	11,11,12	0.54	0	15,15,17	0.97	1 (6%)
2	NAG	m	1	1,2	14,14,15	0.72	0	17,19,21	1.24	2 (11%)
2	NAG	m	2	2	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
2	YZT	m	3	2	13,14,15	1.13	1 (7%)	18,21,23	1.34	2 (11%)
2	BGC	m	4	2	11,11,12	0.86	1 (9%)	15,15,17	1.33	3 (20%)
2	MAN	m	5	2	11,11,12	0.48	0	15,15,17	0.96	0
2	MAN	m	6	2	11,11,12	0.47	0	15,15,17	1.01	0
2	NAG	n	1	1,2	14,14,15	0.39	0	17,19,21	0.80	0
2	NAG	n	2	2	14,14,15	0.55	0	17,19,21	0.85	1 (5%)
2	YZT	n	3	2	13,14,15	1.20	1 (7%)	18,21,23	1.18	1 (5%)
2	BGC	n	4	2	11,11,12	0.25	0	15,15,17	1.11	1 (6%)
2	MAN	n	5	2	11,11,12	0.42	0	15,15,17	0.73	0
2	MAN	n	6	2	11,11,12	0.40	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	o	1	3,1	14,14,15	0.68	0	17,19,21	0.97	1 (5%)
3	NAG	o	2	3	14,14,15	0.50	0	17,19,21	1.77	5 (29%)
3	YZT	o	3	3	13,14,15	1.04	1 (7%)	18,21,23	1.35	3 (16%)
3	MAN	o	4	3	11,11,12	0.84	0	15,15,17	2.70	5 (33%)
2	NAG	p	1	1,2	14,14,15	0.84	0	17,19,21	1.05	1 (5%)
2	NAG	p	2	2	14,14,15	0.56	0	17,19,21	1.07	1 (5%)
2	YZT	p	3	2	13,14,15	1.36	2 (15%)	18,21,23	1.61	3 (16%)
2	BGC	p	4	2	11,11,12	0.97	1 (9%)	15,15,17	2.06	7 (46%)
2	MAN	p	5	2	11,11,12	0.51	0	15,15,17	1.16	2 (13%)
2	MAN	p	6	2	11,11,12	0.54	0	15,15,17	1.13	1 (6%)
2	NAG	q	1	1,2	14,14,15	1.51	2 (14%)	17,19,21	1.99	4 (23%)
2	NAG	q	2	2	14,14,15	0.55	0	17,19,21	1.91	5 (29%)
2	YZT	q	3	2	13,14,15	1.26	1 (7%)	18,21,23	1.96	3 (16%)
2	BGC	q	4	2	11,11,12	0.30	0	15,15,17	1.24	2 (13%)
2	MAN	q	5	2	11,11,12	0.51	0	15,15,17	0.71	0
2	MAN	q	6	2	11,11,12	0.54	0	15,15,17	0.97	1 (6%)
2	NAG	r	1	1,2	14,14,15	0.73	0	17,19,21	1.15	1 (5%)
2	NAG	r	2	2	14,14,15	0.45	0	17,19,21	0.93	1 (5%)
2	YZT	r	3	2	13,14,15	1.13	1 (7%)	18,21,23	1.36	2 (11%)
2	BGC	r	4	2	11,11,12	0.84	1 (9%)	15,15,17	1.34	3 (20%)
2	MAN	r	5	2	11,11,12	0.49	0	15,15,17	0.96	0
2	MAN	r	6	2	11,11,12	0.47	0	15,15,17	1.02	0
2	NAG	s	1	1,2	14,14,15	0.51	0	17,19,21	0.76	0
2	NAG	s	2	2	14,14,15	0.50	0	17,19,21	0.83	1 (5%)
2	YZT	s	3	2	13,14,15	1.18	1 (7%)	18,21,23	1.15	1 (5%)
2	BGC	s	4	2	11,11,12	0.24	0	15,15,17	1.08	2 (13%)
2	MAN	s	5	2	11,11,12	0.44	0	15,15,17	0.72	0
2	MAN	s	6	2	11,11,12	0.42	0	15,15,17	0.80	0
3	NAG	t	1	3,1	14,14,15	0.61	0	17,19,21	1.01	1 (5%)
3	NAG	t	2	3	14,14,15	0.47	0	17,19,21	1.75	5 (29%)
3	YZT	t	3	3	13,14,15	1.05	1 (7%)	18,21,23	1.36	3 (16%)
3	MAN	t	4	3	11,11,12	0.82	0	15,15,17	2.71	5 (33%)
2	NAG	u	1	1,2	14,14,15	0.66	0	17,19,21	0.88	0
2	NAG	u	2	2	14,14,15	0.56	0	17,19,21	1.06	1 (5%)
2	YZT	u	3	2	13,14,15	1.31	2 (15%)	18,21,23	1.60	3 (16%)
2	BGC	u	4	2	11,11,12	0.96	1 (9%)	15,15,17	2.07	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	u	5	2	11,11,12	0.47	0	15,15,17	1.12	2 (13%)
2	MAN	u	6	2	11,11,12	0.53	0	15,15,17	1.11	1 (6%)
2	NAG	v	1	1,2	14,14,15	1.34	2 (14%)	17,19,21	1.81	4 (23%)
2	NAG	v	2	2	14,14,15	0.50	0	17,19,21	1.96	5 (29%)
2	YZT	v	3	2	13,14,15	1.21	1 (7%)	18,21,23	1.96	3 (16%)
2	BGC	v	4	2	11,11,12	0.29	0	15,15,17	1.25	2 (13%)
2	MAN	v	5	2	11,11,12	0.49	0	15,15,17	0.71	0
2	MAN	v	6	2	11,11,12	0.53	0	15,15,17	0.96	1 (6%)
2	NAG	w	1	1,2	14,14,15	0.73	0	17,19,21	1.13	2 (11%)
2	NAG	w	2	2	14,14,15	0.46	0	17,19,21	0.93	1 (5%)
2	YZT	w	3	2	13,14,15	1.13	1 (7%)	18,21,23	1.37	2 (11%)
2	BGC	w	4	2	11,11,12	0.84	1 (9%)	15,15,17	1.35	3 (20%)
2	MAN	w	5	2	11,11,12	0.48	0	15,15,17	0.96	0
2	MAN	w	6	2	11,11,12	0.48	0	15,15,17	1.02	0
2	NAG	x	1	1,2	14,14,15	0.29	0	17,19,21	0.64	0
2	NAG	x	2	2	14,14,15	0.42	0	17,19,21	0.69	0
2	YZT	x	3	2	13,14,15	1.16	1 (7%)	18,21,23	1.15	2 (11%)
2	BGC	x	4	2	11,11,12	0.26	0	15,15,17	1.06	1 (6%)
2	MAN	x	5	2	11,11,12	0.44	0	15,15,17	0.71	0
2	MAN	x	6	2	11,11,12	0.44	0	15,15,17	0.81	0
3	NAG	y	1	3,1	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
3	NAG	y	2	3	14,14,15	0.47	0	17,19,21	1.74	5 (29%)
3	YZT	y	3	3	13,14,15	1.04	1 (7%)	18,21,23	1.35	3 (16%)
3	MAN	y	4	3	11,11,12	0.82	0	15,15,17	2.71	5 (33%)
2	NAG	z	1	1,2	14,14,15	0.48	0	17,19,21	0.82	1 (5%)
2	NAG	z	2	2	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
2	YZT	z	3	2	13,14,15	1.32	2 (15%)	18,21,23	1.58	3 (16%)
2	BGC	z	4	2	11,11,12	0.96	1 (9%)	15,15,17	2.06	6 (40%)
2	MAN	z	5	2	11,11,12	0.49	0	15,15,17	1.12	2 (13%)
2	MAN	z	6	2	11,11,12	0.53	0	15,15,17	1.07	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	0	2	2	-	0/6/23/26	0/1/1/1
2	YZT	0	3	2	-	1/5/22/25	0/1/1/1
2	BGC	0	4	2	-	0/2/19/22	0/1/1/1
2	MAN	0	5	2	-	0/2/19/22	0/1/1/1
2	MAN	0	6	2	-	0/2/19/22	0/1/1/1
2	NAG	1	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	1	2	2	-	2/6/23/26	0/1/1/1
2	YZT	1	3	2	-	0/5/22/25	0/1/1/1
2	BGC	1	4	2	-	0/2/19/22	0/1/1/1
2	MAN	1	5	2	-	0/2/19/22	0/1/1/1
2	MAN	1	6	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	YZT	J	3	2	-	0/5/22/25	0/1/1/1
2	BGC	J	4	2	-	0/2/19/22	0/1/1/1
2	MAN	J	5	2	-	0/2/19/22	0/1/1/1
2	MAN	J	6	2	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	YZT	K	3	3	-	0/5/22/25	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	YZT	L	3	2	-	0/5/22/25	0/1/1/1
2	BGC	L	4	2	-	0/2/19/22	0/1/1/1
2	MAN	L	5	2	-	0/2/19/22	1/1/1/1
2	MAN	L	6	2	-	0/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	YZT	M	3	2	-	1/5/22/25	0/1/1/1
2	BGC	M	4	2	-	0/2/19/22	0/1/1/1
2	MAN	M	5	2	-	0/2/19/22	0/1/1/1
2	MAN	M	6	2	-	0/2/19/22	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	YZT	N	3	2	-	0/5/22/25	0/1/1/1
2	BGC	N	4	2	-	0/2/19/22	0/1/1/1
2	MAN	N	5	2	-	0/2/19/22	0/1/1/1
2	MAN	N	6	2	-	0/2/19/22	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	YZT	O	3	2	-	0/5/22/25	0/1/1/1
2	BGC	O	4	2	-	0/2/19/22	0/1/1/1
2	MAN	O	5	2	-	0/2/19/22	0/1/1/1
2	MAN	O	6	2	-	0/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	YZT	P	3	3	-	0/5/22/25	0/1/1/1
3	MAN	P	4	3	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	YZT	Q	3	2	-	0/5/22/25	0/1/1/1
2	BGC	Q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	5	2	-	0/2/19/22	1/1/1/1
2	MAN	Q	6	2	-	0/2/19/22	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	YZT	R	3	2	-	1/5/22/25	0/1/1/1
2	BGC	R	4	2	-	0/2/19/22	0/1/1/1
2	MAN	R	5	2	-	0/2/19/22	0/1/1/1
2	MAN	R	6	2	-	0/2/19/22	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	YZT	S	3	2	-	0/5/22/25	0/1/1/1
2	BGC	S	4	2	-	0/2/19/22	0/1/1/1
2	MAN	S	5	2	-	0/2/19/22	0/1/1/1
2	MAN	S	6	2	-	0/2/19/22	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	YZT	T	3	2	-	0/5/22/25	0/1/1/1
2	BGC	T	4	2	-	0/2/19/22	0/1/1/1
2	MAN	T	5	2	-	0/2/19/22	0/1/1/1
2	MAN	T	6	2	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	YZT	U	3	3	-	0/5/22/25	0/1/1/1
3	MAN	U	4	3	-	0/2/19/22	0/1/1/1
2	NAG	V	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	YZT	V	3	2	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	V	4	2	-	0/2/19/22	0/1/1/1
2	MAN	V	5	2	-	0/2/19/22	1/1/1/1
2	MAN	V	6	2	-	0/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	YZT	W	3	2	-	1/5/22/25	0/1/1/1
2	BGC	W	4	2	-	0/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	0/1/1/1
2	MAN	W	6	2	-	0/2/19/22	0/1/1/1
2	NAG	X	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1
2	YZT	X	3	2	-	0/5/22/25	0/1/1/1
2	BGC	X	4	2	-	0/2/19/22	0/1/1/1
2	MAN	X	5	2	-	0/2/19/22	0/1/1/1
2	MAN	X	6	2	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	YZT	Y	3	2	-	0/5/22/25	0/1/1/1
2	BGC	Y	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Y	5	2	-	0/2/19/22	0/1/1/1
2	MAN	Y	6	2	-	0/2/19/22	0/1/1/1
3	NAG	Z	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	3/6/23/26	0/1/1/1
3	YZT	Z	3	3	-	0/5/22/25	0/1/1/1
3	MAN	Z	4	3	-	0/2/19/22	0/1/1/1
2	NAG	a	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	YZT	a	3	2	-	0/5/22/25	0/1/1/1
2	BGC	a	4	2	-	0/2/19/22	0/1/1/1
2	MAN	a	5	2	-	0/2/19/22	1/1/1/1
2	MAN	a	6	2	-	0/2/19/22	0/1/1/1
2	NAG	b	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	YZT	b	3	2	-	1/5/22/25	0/1/1/1
2	BGC	b	4	2	-	0/2/19/22	0/1/1/1
2	MAN	b	5	2	-	0/2/19/22	0/1/1/1
2	MAN	b	6	2	-	0/2/19/22	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	2/6/23/26	0/1/1/1
2	YZT	c	3	2	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	c	4	2	-	0/2/19/22	0/1/1/1
2	MAN	c	5	2	-	0/2/19/22	0/1/1/1
2	MAN	c	6	2	-	0/2/19/22	0/1/1/1
2	NAG	d	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1
2	YZT	d	3	2	-	0/5/22/25	0/1/1/1
2	BGC	d	4	2	-	0/2/19/22	0/1/1/1
2	MAN	d	5	2	-	0/2/19/22	0/1/1/1
2	MAN	d	6	2	-	0/2/19/22	0/1/1/1
3	NAG	e	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	3/6/23/26	0/1/1/1
3	YZT	e	3	3	-	0/5/22/25	0/1/1/1
3	MAN	e	4	3	-	0/2/19/22	0/1/1/1
2	NAG	f	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	YZT	f	3	2	-	0/5/22/25	0/1/1/1
2	BGC	f	4	2	-	0/2/19/22	0/1/1/1
2	MAN	f	5	2	-	0/2/19/22	1/1/1/1
2	MAN	f	6	2	-	0/2/19/22	0/1/1/1
2	NAG	g	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	YZT	g	3	2	-	1/5/22/25	0/1/1/1
2	BGC	g	4	2	-	0/2/19/22	0/1/1/1
2	MAN	g	5	2	-	0/2/19/22	0/1/1/1
2	MAN	g	6	2	-	0/2/19/22	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	YZT	h	3	2	-	0/5/22/25	0/1/1/1
2	BGC	h	4	2	-	0/2/19/22	0/1/1/1
2	MAN	h	5	2	-	0/2/19/22	0/1/1/1
2	MAN	h	6	2	-	0/2/19/22	0/1/1/1
2	NAG	i	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
2	YZT	i	3	2	-	0/5/22/25	0/1/1/1
2	BGC	i	4	2	-	0/2/19/22	0/1/1/1
2	MAN	i	5	2	-	0/2/19/22	0/1/1/1
2	MAN	i	6	2	-	0/2/19/22	0/1/1/1
3	NAG	j	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	3/6/23/26	0/1/1/1
3	YZT	j	3	3	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	j	4	3	-	0/2/19/22	0/1/1/1
2	NAG	k	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	k	2	2	-	0/6/23/26	0/1/1/1
2	YZT	k	3	2	-	0/5/22/25	0/1/1/1
2	BGC	k	4	2	-	0/2/19/22	0/1/1/1
2	MAN	k	5	2	-	0/2/19/22	1/1/1/1
2	MAN	k	6	2	-	0/2/19/22	0/1/1/1
2	NAG	l	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	l	2	2	-	0/6/23/26	0/1/1/1
2	YZT	l	3	2	-	1/5/22/25	0/1/1/1
2	BGC	l	4	2	-	0/2/19/22	0/1/1/1
2	MAN	l	5	2	-	0/2/19/22	0/1/1/1
2	MAN	l	6	2	-	0/2/19/22	0/1/1/1
2	NAG	m	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	YZT	m	3	2	-	0/5/22/25	0/1/1/1
2	BGC	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	m	5	2	-	0/2/19/22	0/1/1/1
2	MAN	m	6	2	-	0/2/19/22	0/1/1/1
2	NAG	n	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	n	2	2	-	2/6/23/26	0/1/1/1
2	YZT	n	3	2	-	0/5/22/25	0/1/1/1
2	BGC	n	4	2	-	0/2/19/22	0/1/1/1
2	MAN	n	5	2	-	0/2/19/22	0/1/1/1
2	MAN	n	6	2	-	0/2/19/22	0/1/1/1
3	NAG	o	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	3/6/23/26	0/1/1/1
3	YZT	o	3	3	-	0/5/22/25	0/1/1/1
3	MAN	o	4	3	-	0/2/19/22	0/1/1/1
2	NAG	p	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	YZT	p	3	2	-	0/5/22/25	0/1/1/1
2	BGC	p	4	2	-	0/2/19/22	0/1/1/1
2	MAN	p	5	2	-	0/2/19/22	1/1/1/1
2	MAN	p	6	2	-	0/2/19/22	0/1/1/1
2	NAG	q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	q	2	2	-	0/6/23/26	0/1/1/1
2	YZT	q	3	2	-	1/5/22/25	0/1/1/1
2	BGC	q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	q	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	q	6	2	-	0/2/19/22	0/1/1/1
2	NAG	r	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	r	2	2	-	2/6/23/26	0/1/1/1
2	YZT	r	3	2	-	0/5/22/25	0/1/1/1
2	BGC	r	4	2	-	0/2/19/22	0/1/1/1
2	MAN	r	5	2	-	0/2/19/22	0/1/1/1
2	MAN	r	6	2	-	0/2/19/22	0/1/1/1
2	NAG	s	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
2	YZT	s	3	2	-	0/5/22/25	0/1/1/1
2	BGC	s	4	2	-	0/2/19/22	0/1/1/1
2	MAN	s	5	2	-	0/2/19/22	0/1/1/1
2	MAN	s	6	2	-	0/2/19/22	0/1/1/1
3	NAG	t	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	t	2	3	-	3/6/23/26	0/1/1/1
3	YZT	t	3	3	-	0/5/22/25	0/1/1/1
3	MAN	t	4	3	-	0/2/19/22	0/1/1/1
2	NAG	u	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	u	2	2	-	0/6/23/26	0/1/1/1
2	YZT	u	3	2	-	0/5/22/25	0/1/1/1
2	BGC	u	4	2	-	0/2/19/22	0/1/1/1
2	MAN	u	5	2	-	0/2/19/22	1/1/1/1
2	MAN	u	6	2	-	0/2/19/22	0/1/1/1
2	NAG	v	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	v	2	2	-	0/6/23/26	0/1/1/1
2	YZT	v	3	2	-	1/5/22/25	0/1/1/1
2	BGC	v	4	2	-	0/2/19/22	0/1/1/1
2	MAN	v	5	2	-	0/2/19/22	0/1/1/1
2	MAN	v	6	2	-	0/2/19/22	0/1/1/1
2	NAG	w	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	w	2	2	-	2/6/23/26	0/1/1/1
2	YZT	w	3	2	-	0/5/22/25	0/1/1/1
2	BGC	w	4	2	-	0/2/19/22	0/1/1/1
2	MAN	w	5	2	-	0/2/19/22	0/1/1/1
2	MAN	w	6	2	-	0/2/19/22	0/1/1/1
2	NAG	x	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	x	2	2	-	2/6/23/26	0/1/1/1
2	YZT	x	3	2	-	0/5/22/25	0/1/1/1
2	BGC	x	4	2	-	0/2/19/22	0/1/1/1
2	MAN	x	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	x	6	2	-	0/2/19/22	0/1/1/1
3	NAG	y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	y	2	3	-	3/6/23/26	0/1/1/1
3	YZT	y	3	3	-	0/5/22/25	0/1/1/1
3	MAN	y	4	3	-	0/2/19/22	0/1/1/1
2	NAG	z	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	z	2	2	-	0/6/23/26	0/1/1/1
2	YZT	z	3	2	-	0/5/22/25	0/1/1/1
2	BGC	z	4	2	-	0/2/19/22	0/1/1/1
2	MAN	z	5	2	-	0/2/19/22	1/1/1/1
2	MAN	z	6	2	-	0/2/19/22	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	3	YZT	O2S6-S6	4.70	1.58	1.45
2	Y	3	YZT	O2S6-S6	4.27	1.57	1.45
2	W	3	YZT	O2S6-S6	4.21	1.57	1.45
2	i	3	YZT	O2S6-S6	4.17	1.57	1.45
2	q	3	YZT	O2S6-S6	4.16	1.57	1.45
2	O	3	YZT	O2S6-S6	4.14	1.57	1.45
2	l	3	YZT	O2S6-S6	4.11	1.57	1.45
2	T	3	YZT	O2S6-S6	4.07	1.57	1.45
2	J	3	YZT	O2S6-S6	4.05	1.57	1.45
2	b	3	YZT	O2S6-S6	4.04	1.57	1.45
2	q	1	NAG	O5-C1	-3.98	1.37	1.43
2	M	3	YZT	O2S6-S6	3.94	1.56	1.45
2	v	3	YZT	O2S6-S6	3.94	1.56	1.45
2	n	3	YZT	O2S6-S6	3.90	1.56	1.45
2	R	3	YZT	O2S6-S6	3.84	1.56	1.45
2	x	3	YZT	O2S6-S6	3.82	1.56	1.45
2	s	3	YZT	O2S6-S6	3.82	1.56	1.45
2	g	3	YZT	O2S6-S6	3.81	1.56	1.45
2	k	3	YZT	O2S6-S6	3.69	1.55	1.45
2	S	3	YZT	O2S6-S6	3.62	1.55	1.45
2	l	3	YZT	O2S6-S6	3.61	1.55	1.45
2	p	3	YZT	O2S6-S6	3.61	1.55	1.45
2	w	3	YZT	O2S6-S6	3.55	1.55	1.45
2	N	3	YZT	O2S6-S6	3.54	1.55	1.45
2	0	3	YZT	O2S6-S6	3.54	1.55	1.45
2	m	3	YZT	O2S6-S6	3.53	1.55	1.45
2	X	3	YZT	O2S6-S6	3.52	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	3	YZT	O2S6-S6	3.51	1.55	1.45
2	h	3	YZT	O2S6-S6	3.51	1.55	1.45
2	a	3	YZT	O2S6-S6	3.50	1.55	1.45
2	c	3	YZT	O2S6-S6	3.49	1.55	1.45
2	u	3	YZT	O2S6-S6	3.46	1.55	1.45
2	V	3	YZT	O2S6-S6	3.44	1.55	1.45
2	z	3	YZT	O2S6-S6	3.44	1.55	1.45
2	L	3	YZT	O2S6-S6	3.41	1.55	1.45
2	f	3	YZT	O2S6-S6	3.40	1.55	1.45
2	Q	3	YZT	O2S6-S6	3.25	1.54	1.45
2	v	1	NAG	O5-C1	-3.19	1.38	1.43
3	U	3	YZT	O2S6-S6	3.16	1.54	1.45
3	j	3	YZT	O2S6-S6	3.15	1.54	1.45
3	P	3	YZT	O2S6-S6	3.15	1.54	1.45
3	Z	3	YZT	O2S6-S6	3.15	1.54	1.45
3	e	3	YZT	O2S6-S6	3.15	1.54	1.45
3	K	3	YZT	O2S6-S6	3.12	1.54	1.45
3	t	3	YZT	O2S6-S6	3.12	1.54	1.45
3	o	3	YZT	O2S6-S6	3.11	1.54	1.45
3	y	3	YZT	O2S6-S6	3.09	1.54	1.45
2	M	1	NAG	O5-C1	-2.99	1.38	1.43
2	l	1	NAG	O5-C1	-2.81	1.39	1.43
2	W	1	NAG	C1-C2	-2.66	1.48	1.52
2	q	1	NAG	C1-C2	-2.66	1.48	1.52
2	v	1	NAG	C1-C2	-2.59	1.48	1.52
2	f	4	BGC	O5-C1	-2.55	1.39	1.43
2	k	4	BGC	O5-C1	-2.50	1.39	1.43
2	u	4	BGC	O5-C1	-2.49	1.39	1.43
2	b	1	NAG	O5-C1	-2.48	1.39	1.43
2	p	4	BGC	O5-C1	-2.48	1.39	1.43
2	Q	4	BGC	O5-C1	-2.48	1.39	1.43
2	L	4	BGC	O5-C1	-2.46	1.39	1.43
2	R	1	NAG	C1-C2	-2.46	1.48	1.52
2	V	4	BGC	O5-C1	-2.45	1.39	1.43
2	z	4	BGC	O5-C1	-2.44	1.39	1.43
2	a	4	BGC	O5-C1	-2.42	1.39	1.43
2	M	1	NAG	C1-C2	-2.31	1.48	1.52
2	R	1	NAG	O5-C1	-2.28	1.40	1.43
2	Q	3	YZT	O5-C1	-2.25	1.40	1.43
2	l	4	BGC	O5-C1	-2.24	1.40	1.43
2	N	4	BGC	O5-C1	-2.24	1.40	1.43
2	m	4	BGC	O5-C1	-2.22	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	z	3	YZT	O5-C1	-2.21	1.40	1.43
2	S	4	BGC	O5-C1	-2.19	1.40	1.43
2	X	4	BGC	O5-C1	-2.18	1.40	1.43
2	h	4	BGC	O5-C1	-2.18	1.40	1.43
2	k	3	YZT	O5-C1	-2.17	1.40	1.43
2	w	4	BGC	O5-C1	-2.17	1.40	1.43
2	r	4	BGC	O5-C1	-2.14	1.40	1.43
2	c	4	BGC	O5-C1	-2.13	1.40	1.43
2	a	3	YZT	O5-C1	-2.13	1.40	1.43
2	g	1	NAG	O5-C1	-2.13	1.40	1.43
2	b	1	NAG	C1-C2	-2.13	1.49	1.52
2	p	3	YZT	O5-C1	-2.13	1.40	1.43
2	W	1	NAG	O5-C1	-2.12	1.40	1.43
2	L	3	YZT	O5-C1	-2.09	1.40	1.43
2	V	3	YZT	O5-C1	-2.06	1.40	1.43
2	u	3	YZT	O5-C1	-2.02	1.40	1.43

All (488) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	3	YZT	O2S6-S6-C6	-7.07	98.54	106.94
2	M	3	YZT	O2S6-S6-C6	-7.06	98.55	106.94
2	q	3	YZT	O2S6-S6-C6	-6.79	98.87	106.94
2	v	3	YZT	O2S6-S6-C6	-6.78	98.88	106.94
2	b	3	YZT	O2S6-S6-C6	-6.77	98.90	106.94
2	W	3	YZT	O2S6-S6-C6	-6.77	98.90	106.94
3	y	4	MAN	O2-C2-C1	-6.71	95.42	109.15
3	t	4	MAN	O2-C2-C1	-6.71	95.43	109.15
3	K	4	MAN	O2-C2-C1	-6.69	95.47	109.15
3	P	4	MAN	O2-C2-C1	-6.68	95.49	109.15
3	j	4	MAN	O2-C2-C1	-6.66	95.53	109.15
3	U	4	MAN	O2-C2-C1	-6.64	95.56	109.15
3	o	4	MAN	O2-C2-C1	-6.64	95.57	109.15
3	e	4	MAN	O2-C2-C1	-6.63	95.58	109.15
3	Z	4	MAN	O2-C2-C1	-6.63	95.59	109.15
2	g	3	YZT	O2S6-S6-C6	-6.61	99.08	106.94
2	0	3	YZT	O2S6-S6-C6	-6.32	99.43	106.94
2	R	3	YZT	O2S6-S6-C6	-6.30	99.45	106.94
3	K	4	MAN	O5-C1-C2	5.83	119.77	110.77
3	j	4	MAN	O5-C1-C2	5.81	119.74	110.77
3	t	4	MAN	O5-C1-C2	5.81	119.73	110.77
3	P	4	MAN	O5-C1-C2	5.79	119.71	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	y	4	MAN	O5-C1-C2	5.79	119.71	110.77
3	e	4	MAN	O5-C1-C2	5.78	119.70	110.77
3	U	4	MAN	O5-C1-C2	5.78	119.69	110.77
3	o	4	MAN	O5-C1-C2	5.77	119.67	110.77
3	Z	4	MAN	O5-C1-C2	5.74	119.64	110.77
2	M	2	NAG	C1-O5-C5	5.62	119.80	112.19
2	R	2	NAG	C1-O5-C5	5.55	119.71	112.19
2	v	2	NAG	C1-O5-C5	5.36	119.46	112.19
2	b	2	NAG	C1-O5-C5	5.22	119.26	112.19
2	W	2	NAG	C1-O5-C5	5.21	119.25	112.19
2	0	2	NAG	C1-O5-C5	5.14	119.15	112.19
2	q	2	NAG	C1-O5-C5	5.13	119.15	112.19
2	l	2	NAG	C1-O5-C5	5.03	119.01	112.19
2	q	1	NAG	C1-O5-C5	4.97	118.92	112.19
2	g	2	NAG	C1-O5-C5	4.94	118.89	112.19
2	f	4	BGC	C1-C2-C3	4.55	115.26	109.67
2	L	4	BGC	C1-C2-C3	4.54	115.24	109.67
2	k	4	BGC	C1-C2-C3	4.54	115.24	109.67
2	z	4	BGC	C1-C2-C3	4.51	115.21	109.67
2	a	4	BGC	C1-C2-C3	4.51	115.20	109.67
2	u	4	BGC	C1-C2-C3	4.50	115.19	109.67
2	p	4	BGC	C1-C2-C3	4.49	115.18	109.67
2	Q	4	BGC	C1-C2-C3	4.48	115.17	109.67
2	V	4	BGC	C1-C2-C3	4.46	115.15	109.67
2	v	1	NAG	C1-O5-C5	4.34	118.08	112.19
2	u	3	YZT	O5-C1-C2	-4.05	104.53	110.77
2	f	3	YZT	O5-C1-C2	-4.03	104.55	110.77
2	S	3	YZT	O2S6-S6-C6	-4.02	102.17	106.94
2	L	3	YZT	O5-C1-C2	-4.00	104.59	110.77
2	V	3	YZT	O5-C1-C2	-3.99	104.61	110.77
2	k	3	YZT	O5-C1-C2	-3.96	104.66	110.77
2	p	3	YZT	O5-C1-C2	-3.95	104.68	110.77
2	a	3	YZT	O5-C1-C2	-3.94	104.69	110.77
2	z	3	YZT	O5-C1-C2	-3.93	104.70	110.77
2	Q	3	YZT	O5-C1-C2	-3.86	104.82	110.77
2	l	3	YZT	O2S6-S6-C6	-3.86	102.36	106.94
2	W	1	NAG	C2-N2-C7	-3.82	117.46	122.90
2	M	4	BGC	C1-O5-C5	3.78	117.31	112.19
2	X	3	YZT	O2S6-S6-C6	-3.77	102.46	106.94
2	g	1	NAG	C2-N2-C7	-3.72	117.60	122.90
2	N	3	YZT	O2S6-S6-C6	-3.66	102.59	106.94
2	w	3	YZT	O2S6-S6-C6	-3.65	102.60	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	1	NAG	C2-N2-C7	-3.62	117.75	122.90
2	b	1	NAG	C2-N2-C7	-3.59	117.79	122.90
2	q	1	NAG	C2-N2-C7	-3.59	117.80	122.90
2	R	1	NAG	C2-N2-C7	-3.58	117.81	122.90
2	W	4	BGC	C1-O5-C5	3.57	117.03	112.19
2	b	4	BGC	C1-O5-C5	3.57	117.02	112.19
2	R	4	BGC	C1-O5-C5	3.56	117.02	112.19
2	v	1	NAG	C2-N2-C7	-3.55	117.85	122.90
2	L	5	MAN	C1-O5-C5	3.55	117.00	112.19
2	g	4	BGC	C1-O5-C5	3.54	117.00	112.19
2	r	3	YZT	O2S6-S6-C6	-3.54	102.73	106.94
2	n	3	YZT	O1S6-S6-O3S6	3.52	119.88	111.27
2	c	3	YZT	O2S6-S6-C6	-3.50	102.78	106.94
2	l	4	BGC	C1-O5-C5	3.50	116.93	112.19
2	h	3	YZT	O2S6-S6-C6	-3.49	102.79	106.94
2	q	4	BGC	C1-O5-C5	3.49	116.92	112.19
2	m	3	YZT	O2S6-S6-C6	-3.48	102.80	106.94
2	v	4	BGC	C1-O5-C5	3.48	116.90	112.19
2	z	5	MAN	C1-O5-C5	3.48	116.90	112.19
2	0	4	BGC	C1-O5-C5	3.45	116.86	112.19
2	a	5	MAN	C1-O5-C5	3.42	116.83	112.19
2	M	1	NAG	C1-O5-C5	3.42	116.83	112.19
2	W	6	MAN	C1-O5-C5	3.42	116.83	112.19
2	u	5	MAN	C1-O5-C5	3.42	116.82	112.19
2	b	3	YZT	O5-C1-C2	-3.39	105.53	110.77
2	l	6	MAN	C1-O5-C5	3.38	116.78	112.19
2	p	5	MAN	C1-O5-C5	3.38	116.77	112.19
2	Q	5	MAN	C1-O5-C5	3.38	116.77	112.19
2	k	5	MAN	C1-O5-C5	3.36	116.75	112.19
2	q	6	MAN	C1-O5-C5	3.36	116.74	112.19
2	T	3	YZT	O1S6-S6-O3S6	3.36	119.48	111.27
2	W	3	YZT	O5-C1-C2	-3.35	105.60	110.77
2	s	3	YZT	O1S6-S6-O3S6	3.34	119.42	111.27
2	V	5	MAN	C1-O5-C5	3.33	116.71	112.19
2	R	6	MAN	C1-O5-C5	3.33	116.70	112.19
2	g	6	MAN	C1-O5-C5	3.33	116.70	112.19
2	f	5	MAN	C1-O5-C5	3.32	116.69	112.19
2	b	6	MAN	C1-O5-C5	3.32	116.69	112.19
2	v	6	MAN	C1-O5-C5	3.30	116.66	112.19
2	q	3	YZT	O5-C1-C2	-3.30	105.68	110.77
2	M	6	MAN	C1-O5-C5	3.30	116.66	112.19
2	Q	3	YZT	O1S6-S6-O3S6	3.25	119.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	t	3	YZT	O1S6-S6-O3S6	3.25	119.21	111.27
2	g	3	YZT	O5-C1-C2	-3.25	105.76	110.77
3	K	3	YZT	O1S6-S6-O3S6	3.25	119.20	111.27
3	P	3	YZT	O1S6-S6-O3S6	3.24	119.20	111.27
2	f	3	YZT	O2S6-S6-C6	-3.24	103.09	106.94
3	U	3	YZT	O1S6-S6-O3S6	3.24	119.19	111.27
2	M	1	NAG	C2-N2-C7	-3.23	118.30	122.90
3	j	3	YZT	O1S6-S6-O3S6	3.23	119.17	111.27
2	S	4	BGC	C1-C2-C3	3.23	113.64	109.67
3	o	2	NAG	C2-N2-C7	3.23	127.50	122.90
2	l	3	YZT	O5-C1-C2	-3.23	105.79	110.77
2	v	3	YZT	O5-C1-C2	-3.22	105.79	110.77
3	y	3	YZT	O1S6-S6-O3S6	3.22	119.15	111.27
2	N	4	BGC	C1-C2-C3	3.22	113.62	109.67
3	Z	3	YZT	O1S6-S6-O3S6	3.22	119.13	111.27
2	k	3	YZT	O1S6-S6-O3S6	3.21	119.12	111.27
3	j	2	NAG	C2-N2-C7	3.21	127.48	122.90
2	n	4	BGC	C1-O5-C5	3.21	116.54	112.19
3	o	3	YZT	O1S6-S6-O3S6	3.21	119.11	111.27
2	k	4	BGC	C6-C5-C4	-3.21	105.49	113.00
2	l	4	BGC	C1-C2-C3	3.21	113.61	109.67
2	f	4	BGC	C6-C5-C4	-3.20	105.50	113.00
2	r	4	BGC	C1-C2-C3	3.20	113.60	109.67
3	U	2	NAG	C2-N2-C7	3.20	127.46	122.90
2	L	3	YZT	O1S6-S6-O3S6	3.20	119.09	111.27
3	e	3	YZT	O1S6-S6-O3S6	3.20	119.09	111.27
2	R	3	YZT	O5-C1-C2	-3.20	105.84	110.77
2	w	4	BGC	C1-C2-C3	3.19	113.59	109.67
2	u	4	BGC	C6-C5-C4	-3.19	105.52	113.00
2	d	4	BGC	C1-O5-C5	3.19	116.51	112.19
2	T	4	BGC	C1-O5-C5	3.19	116.51	112.19
3	e	2	NAG	C2-N2-C7	3.18	127.44	122.90
2	p	4	BGC	C6-C5-C4	-3.18	105.55	113.00
2	0	6	MAN	C1-O5-C5	3.18	116.50	112.19
2	h	4	BGC	C1-C2-C3	3.18	113.58	109.67
2	X	4	BGC	C1-C2-C3	3.18	113.57	109.67
2	L	4	BGC	C6-C5-C4	-3.18	105.56	113.00
2	c	4	BGC	C1-C2-C3	3.18	113.57	109.67
2	m	4	BGC	C1-C2-C3	3.18	113.57	109.67
2	l	1	NAG	C1-O5-C5	3.18	116.50	112.19
3	Z	2	NAG	C2-N2-C7	3.17	127.42	122.90
2	a	4	BGC	C6-C5-C4	-3.17	105.59	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	NAG	C2-N2-C7	3.16	127.41	122.90
2	Q	4	BGC	C6-C5-C4	-3.16	105.59	113.00
2	z	4	BGC	C6-C5-C4	-3.16	105.61	113.00
2	i	4	BGC	C1-O5-C5	3.16	116.47	112.19
2	V	4	BGC	C6-C5-C4	-3.15	105.62	113.00
2	V	3	YZT	O1S6-S6-O3S6	3.14	118.96	111.27
2	N	1	NAG	O5-C1-C2	-3.14	106.34	111.29
3	K	2	NAG	C2-N2-C7	3.13	127.36	122.90
3	Z	4	MAN	C1-C2-C3	3.13	113.52	109.67
2	u	3	YZT	O1S6-S6-O3S6	3.12	118.90	111.27
2	z	3	YZT	O1S6-S6-O3S6	3.12	118.90	111.27
3	t	2	NAG	C2-N2-C7	3.12	127.34	122.90
2	p	3	YZT	O1S6-S6-O3S6	3.12	118.89	111.27
2	Y	3	YZT	O1S6-S6-O3S6	3.11	118.88	111.27
3	o	4	MAN	C1-C2-C3	3.11	113.49	109.67
3	U	4	MAN	C1-C2-C3	3.11	113.49	109.67
3	P	4	MAN	C1-C2-C3	3.09	113.46	109.67
3	e	4	MAN	C1-C2-C3	3.09	113.46	109.67
2	a	3	YZT	O1S6-S6-O3S6	3.09	118.81	111.27
3	j	4	MAN	C1-C2-C3	3.08	113.46	109.67
2	O	4	BGC	C1-O5-C5	3.08	116.36	112.19
3	t	4	MAN	C1-C2-C3	3.07	113.44	109.67
3	y	4	MAN	C1-C2-C3	3.07	113.44	109.67
2	s	4	BGC	C1-O5-C5	3.06	116.33	112.19
2	q	1	NAG	O3-C3-C2	3.05	115.77	109.47
3	K	4	MAN	C1-C2-C3	3.05	113.41	109.67
2	Y	4	BGC	C1-O5-C5	3.04	116.31	112.19
3	y	2	NAG	C2-N2-C7	3.04	127.24	122.90
2	i	3	YZT	O1S6-S6-O3S6	3.04	118.70	111.27
2	f	3	YZT	O1S6-S6-O3S6	3.03	118.68	111.27
3	y	1	NAG	O5-C1-C2	-3.02	106.53	111.29
2	c	3	YZT	O1S6-S6-O3S6	3.01	118.64	111.27
2	M	3	YZT	O5-C1-C2	-3.01	106.12	110.77
2	0	1	NAG	C2-N2-C7	-3.00	118.64	122.90
3	o	2	NAG	C1-O5-C5	-3.00	108.13	112.19
3	e	2	NAG	C1-O5-C5	-2.99	108.14	112.19
2	h	3	YZT	O1S6-S6-O3S6	2.99	118.58	111.27
3	j	2	NAG	C1-O5-C5	-2.98	108.15	112.19
3	P	2	NAG	C1-O5-C5	-2.98	108.15	112.19
3	Z	2	NAG	C1-O5-C5	-2.98	108.16	112.19
3	U	2	NAG	C1-O5-C5	-2.97	108.16	112.19
2	x	4	BGC	C1-O5-C5	2.97	116.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	3	YZT	O1S6-S6-O3S6	2.96	118.52	111.27
2	l	1	NAG	O3-C3-C2	2.96	115.59	109.47
2	r	3	YZT	O1S6-S6-O3S6	2.96	118.50	111.27
3	K	2	NAG	C1-O5-C5	-2.96	108.19	112.19
2	m	3	YZT	O1S6-S6-O3S6	2.94	118.47	111.27
2	J	4	BGC	C1-O5-C5	2.94	116.17	112.19
3	y	2	NAG	C1-O5-C5	-2.93	108.23	112.19
2	N	3	YZT	O1S6-S6-O3S6	2.92	118.41	111.27
2	w	3	YZT	O1S6-S6-O3S6	2.92	118.40	111.27
3	t	2	NAG	C1-O5-C5	-2.92	108.24	112.19
2	0	3	YZT	O1S6-S6-O3S6	2.91	118.40	111.27
2	b	1	NAG	C1-O5-C5	2.90	116.12	112.19
2	X	3	YZT	O1S6-S6-O3S6	2.89	118.34	111.27
2	0	3	YZT	O5-C1-C2	-2.88	106.32	110.77
2	h	1	NAG	O5-C1-C2	-2.88	106.75	111.29
2	1	3	YZT	O1S6-S6-O3S6	2.88	118.30	111.27
2	S	3	YZT	O1S6-S6-O3S6	2.85	118.24	111.27
2	c	1	NAG	C2-N2-C7	-2.84	118.86	122.90
3	P	2	NAG	C3-C4-C5	2.82	115.28	110.24
3	t	1	NAG	O5-C1-C2	-2.82	106.83	111.29
3	Z	2	NAG	C3-C4-C5	2.81	115.26	110.24
3	o	2	NAG	C3-C4-C5	2.81	115.25	110.24
2	R	1	NAG	C1-O5-C5	2.80	115.98	112.19
3	j	2	NAG	C3-C4-C5	2.80	115.23	110.24
2	W	2	NAG	C4-C3-C2	2.80	115.12	111.02
2	b	2	NAG	C4-C3-C2	2.80	115.11	111.02
3	K	2	NAG	C3-C4-C5	2.79	115.22	110.24
3	e	2	NAG	C3-C4-C5	2.79	115.22	110.24
3	y	2	NAG	C3-C4-C5	2.79	115.22	110.24
3	t	2	NAG	C3-C4-C5	2.79	115.21	110.24
3	U	2	NAG	C3-C4-C5	2.78	115.20	110.24
2	v	2	NAG	C4-C3-C2	2.77	115.08	111.02
2	R	2	NAG	C4-C3-C2	2.76	115.07	111.02
2	M	2	NAG	C4-C3-C2	2.76	115.06	111.02
2	Q	2	NAG	O3-C3-C4	-2.75	103.98	110.35
2	h	1	NAG	C2-N2-C7	-2.75	118.99	122.90
2	M	1	NAG	O3-C3-C2	2.75	115.16	109.47
3	e	1	NAG	O5-C1-C2	-2.75	106.95	111.29
2	0	2	NAG	C4-C3-C2	2.75	115.05	111.02
3	P	1	NAG	O5-C1-C2	-2.74	106.96	111.29
2	x	3	YZT	O1S6-S6-O3S6	2.74	117.96	111.27
2	q	2	NAG	C4-C3-C2	2.73	115.03	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	1	NAG	O5-C1-C2	-2.73	106.97	111.29
2	W	1	NAG	O3-C3-C2	2.73	115.11	109.47
2	J	3	YZT	O1S6-S6-O3S6	2.72	117.92	111.27
2	g	1	NAG	O3-C3-C2	2.71	115.08	109.47
2	l	2	NAG	C4-C3-C2	2.71	114.99	111.02
3	o	1	NAG	O5-C1-C2	-2.71	107.01	111.29
2	f	4	BGC	O3-C3-C4	-2.71	104.09	110.35
2	k	4	BGC	O3-C3-C4	-2.71	104.09	110.35
2	N	1	NAG	C2-N2-C7	-2.71	119.05	122.90
2	g	2	NAG	C4-C3-C2	2.70	114.98	111.02
3	Z	4	MAN	C3-C4-C5	2.70	115.05	110.24
2	V	2	NAG	O3-C3-C4	-2.70	104.11	110.35
2	L	2	NAG	O3-C3-C4	-2.70	104.12	110.35
2	k	1	NAG	O5-C1-C2	-2.69	107.03	111.29
3	U	1	NAG	O5-C1-C2	-2.69	107.04	111.29
3	j	1	NAG	O5-C1-C2	-2.69	107.04	111.29
2	u	4	BGC	O3-C3-C4	-2.69	104.14	110.35
2	p	4	BGC	O3-C3-C4	-2.69	104.14	110.35
2	L	4	BGC	O3-C3-C4	-2.68	104.16	110.35
3	y	2	NAG	C4-C3-C2	2.68	114.94	111.02
2	W	1	NAG	C1-O5-C5	2.68	115.82	112.19
2	z	4	BGC	O2-C2-C1	-2.67	103.69	109.15
2	V	4	BGC	O3-C3-C4	-2.67	104.18	110.35
3	j	2	NAG	C4-C3-C2	2.67	114.93	111.02
2	z	4	BGC	O3-C3-C4	-2.67	104.18	110.35
2	b	1	NAG	O3-C3-C2	2.67	114.98	109.47
3	o	4	MAN	C3-C4-C5	2.67	114.99	110.24
3	Z	2	NAG	C4-C3-C2	2.66	114.92	111.02
3	Z	1	NAG	O5-C1-C2	-2.66	107.08	111.29
3	U	2	NAG	C4-C3-C2	2.66	114.92	111.02
3	o	2	NAG	C4-C3-C2	2.66	114.92	111.02
3	U	4	MAN	C3-C4-C5	2.66	114.98	110.24
3	t	2	NAG	C4-C3-C2	2.66	114.91	111.02
2	p	3	YZT	O2S6-S6-C6	-2.66	103.78	106.94
3	K	1	NAG	O5-C1-C2	-2.65	107.10	111.29
2	u	2	NAG	O3-C3-C4	-2.65	104.22	110.35
3	e	2	NAG	C4-C3-C2	2.65	114.90	111.02
2	a	4	BGC	O3-C3-C4	-2.64	104.24	110.35
2	u	4	BGC	O2-C2-C1	-2.64	103.75	109.15
3	y	2	NAG	O5-C5-C6	2.64	111.34	107.20
3	e	4	MAN	C3-C4-C5	2.64	114.95	110.24
2	R	1	NAG	O3-C3-C2	2.64	114.93	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	4	MAN	C3-C4-C5	2.64	114.95	110.24
2	Q	4	BGC	O3-C3-C4	-2.64	104.25	110.35
3	K	2	NAG	C4-C3-C2	2.64	114.88	111.02
3	P	2	NAG	C4-C3-C2	2.64	114.88	111.02
2	f	2	NAG	O3-C3-C4	-2.63	104.27	110.35
2	a	4	BGC	O2-C2-C1	-2.63	103.77	109.15
2	V	4	BGC	O2-C2-C1	-2.63	103.78	109.15
3	j	4	MAN	C3-C4-C5	2.63	114.92	110.24
2	L	4	BGC	O2-C2-C1	-2.63	103.78	109.15
2	0	2	NAG	O5-C5-C6	-2.62	103.09	107.20
2	p	4	BGC	O2-C2-C1	-2.62	103.79	109.15
2	v	3	YZT	O1S6-S6-O3S6	2.62	117.68	111.27
2	a	2	NAG	O3-C3-C4	-2.62	104.30	110.35
2	p	2	NAG	O3-C3-C4	-2.62	104.30	110.35
3	y	4	MAN	C3-C4-C5	2.62	114.91	110.24
3	K	4	MAN	C3-C4-C5	2.61	114.90	110.24
2	k	2	NAG	O3-C3-C4	-2.60	104.34	110.35
2	f	4	BGC	O2-C2-C1	-2.59	103.84	109.15
2	k	4	BGC	O2-C2-C1	-2.59	103.85	109.15
2	Q	4	BGC	O2-C2-C1	-2.58	103.87	109.15
3	t	2	NAG	O5-C5-C6	2.58	111.25	107.20
3	t	4	MAN	C3-C4-C5	2.58	114.84	110.24
2	k	3	YZT	O2S6-S6-C6	-2.57	103.89	106.94
2	c	1	NAG	O5-C1-C2	-2.56	107.24	111.29
2	z	2	NAG	O3-C3-C4	-2.56	104.42	110.35
2	v	1	NAG	O3-C3-C2	2.56	114.75	109.47
3	K	2	NAG	O5-C5-C6	2.53	111.17	107.20
2	X	1	NAG	C2-N2-C7	-2.52	119.31	122.90
2	g	3	YZT	O1S6-S6-O3S6	2.51	117.41	111.27
2	S	1	NAG	C2-N2-C7	-2.51	119.33	122.90
2	d	3	YZT	O1S6-S6-O3S6	2.50	117.39	111.27
3	P	2	NAG	O5-C5-C6	2.50	111.13	107.20
2	S	1	NAG	O5-C1-C2	-2.50	107.34	111.29
2	a	3	YZT	O2S6-S6-C6	-2.50	103.97	106.94
3	e	2	NAG	O5-C5-C6	2.50	111.12	107.20
2	g	1	NAG	C1-O5-C5	2.49	115.57	112.19
2	M	2	NAG	O5-C5-C6	-2.49	103.30	107.20
2	l	1	NAG	C3-C4-C5	-2.49	105.80	110.24
3	j	2	NAG	O5-C5-C6	2.48	111.10	107.20
2	W	2	NAG	O4-C4-C3	-2.48	104.61	110.35
3	U	2	NAG	O5-C5-C6	2.48	111.09	107.20
3	Z	2	NAG	O5-C5-C6	2.48	111.09	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	1	NAG	C1-O5-C5	2.48	115.55	112.19
2	u	3	YZT	O2S6-S6-C6	-2.48	104.00	106.94
2	b	2	NAG	O4-C4-C3	-2.47	104.64	110.35
2	g	2	NAG	O5-C5-C6	-2.47	103.34	107.20
2	0	1	NAG	O3-C3-C2	2.46	114.56	109.47
3	o	2	NAG	O5-C5-C6	2.46	111.06	107.20
2	q	2	NAG	O4-C4-C3	-2.45	104.68	110.35
2	v	2	NAG	O4-C4-C3	-2.45	104.69	110.35
2	V	1	NAG	O5-C1-C2	-2.45	107.42	111.29
3	e	3	YZT	C1-C2-C3	2.45	112.67	109.67
2	b	2	NAG	O5-C5-C6	-2.44	103.37	107.20
2	R	2	NAG	O4-C4-C3	-2.44	104.72	110.35
3	K	3	YZT	C1-C2-C3	2.43	112.65	109.67
3	U	3	YZT	C1-C2-C3	2.43	112.65	109.67
2	v	2	NAG	O5-C5-C6	-2.42	103.40	107.20
3	j	3	YZT	C1-C2-C3	2.42	112.64	109.67
3	o	3	YZT	C1-C2-C3	2.42	112.64	109.67
2	q	1	NAG	C3-C4-C5	-2.42	105.93	110.24
2	M	4	BGC	C1-C2-C3	2.42	112.64	109.67
3	Z	3	YZT	C1-C2-C3	2.41	112.63	109.67
3	P	3	YZT	C1-C2-C3	2.41	112.63	109.67
2	W	2	NAG	O5-C5-C6	-2.41	103.43	107.20
2	q	2	NAG	O5-C5-C6	-2.41	103.43	107.20
3	t	3	YZT	C1-C2-C3	2.41	112.62	109.67
2	x	3	YZT	O2S6-S6-C6	-2.40	104.09	106.94
2	l	2	NAG	O5-C5-C6	-2.39	103.45	107.20
2	v	4	BGC	C1-C2-C3	2.39	112.61	109.67
2	z	3	YZT	O2S6-S6-C6	-2.39	104.10	106.94
3	y	3	YZT	C1-C2-C3	2.39	112.60	109.67
2	l	2	NAG	O4-C4-C3	-2.39	104.83	110.35
2	b	4	BGC	C1-C2-C3	2.37	112.58	109.67
2	V	3	YZT	O2S6-S6-C6	-2.36	104.13	106.94
2	g	2	NAG	O4-C4-C3	-2.36	104.89	110.35
2	R	3	YZT	O1S6-S6-O3S6	2.36	117.04	111.27
2	k	5	MAN	O5-C1-C2	2.36	114.41	110.77
2	M	2	NAG	O4-C4-C3	-2.36	104.90	110.35
2	0	2	NAG	O4-C4-C3	-2.35	104.93	110.35
2	l	3	YZT	O1S6-S6-O3S6	2.34	116.99	111.27
2	r	1	NAG	O5-C1-C2	-2.34	107.60	111.29
2	R	4	BGC	C1-C2-C3	2.33	112.53	109.67
2	W	4	BGC	C1-C2-C3	2.33	112.53	109.67
2	M	3	YZT	O1S6-S6-O3S6	2.33	116.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	4	BGC	C1-C2-C3	2.32	112.52	109.67
2	k	6	MAN	C1-C2-C3	2.31	112.51	109.67
2	S	4	BGC	O2-C2-C3	-2.31	105.52	110.14
2	q	4	BGC	C1-C2-C3	2.30	112.50	109.67
2	R	2	NAG	O5-C5-C6	-2.30	103.60	107.20
2	l	4	BGC	O2-C2-C3	-2.30	105.53	110.14
2	l	4	BGC	C1-C2-C3	2.30	112.49	109.67
2	Q	1	NAG	O5-C1-C2	-2.30	107.66	111.29
2	r	4	BGC	O2-C2-C3	-2.29	105.54	110.14
2	m	1	NAG	C2-N2-C7	-2.29	119.64	122.90
2	f	6	MAN	C1-C2-C3	2.29	112.48	109.67
2	Q	5	MAN	O5-C1-C2	2.29	114.30	110.77
2	c	4	BGC	O2-C2-C3	-2.28	105.57	110.14
2	w	4	BGC	O2-C2-C3	-2.28	105.57	110.14
2	h	4	BGC	O2-C2-C3	-2.28	105.57	110.14
2	m	4	BGC	O2-C2-C3	-2.28	105.58	110.14
2	f	1	NAG	O5-C1-C2	-2.28	107.69	111.29
2	N	4	BGC	O2-C2-C3	-2.27	105.59	110.14
2	X	4	BGC	O2-C2-C3	-2.27	105.59	110.14
2	w	1	NAG	O5-C1-C2	-2.27	107.71	111.29
2	X	1	NAG	O5-C1-C2	-2.26	107.72	111.29
2	0	4	BGC	C1-C2-C3	2.26	112.44	109.67
3	Z	4	MAN	O3-C3-C2	2.24	114.29	109.99
2	L	5	MAN	O5-C1-C2	2.24	114.23	110.77
2	a	1	NAG	O5-C1-C2	-2.23	107.76	111.29
2	q	3	YZT	O1S6-S6-O3S6	2.23	116.73	111.27
3	U	4	MAN	O3-C3-C2	2.23	114.27	109.99
2	L	3	YZT	O2S6-S6-C6	-2.23	104.29	106.94
3	j	4	MAN	O3-C3-C2	2.23	114.26	109.99
3	o	4	MAN	O3-C3-C2	2.23	114.26	109.99
2	z	1	NAG	O5-C1-C2	-2.23	107.77	111.29
2	Q	3	YZT	O2S6-S6-C6	-2.23	104.29	106.94
2	g	1	NAG	C3-C4-C5	-2.22	106.28	110.24
2	a	4	BGC	O5-C1-C2	-2.22	107.35	110.77
2	p	6	MAN	C1-C2-C3	2.22	112.39	109.67
2	V	4	BGC	O5-C1-C2	-2.22	107.35	110.77
2	L	6	MAN	C1-C2-C3	2.22	112.39	109.67
2	u	4	BGC	O5-C1-C2	-2.21	107.36	110.77
2	p	5	MAN	O5-C1-C2	2.20	114.17	110.77
2	L	4	BGC	O5-C1-C2	-2.20	107.38	110.77
2	k	4	BGC	O5-C1-C2	-2.20	107.38	110.77
2	Q	4	BGC	O5-C1-C2	-2.20	107.38	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	6	MAN	C1-C2-C3	2.19	112.36	109.67
2	a	6	MAN	C1-C2-C3	2.19	112.36	109.67
2	z	4	BGC	O5-C1-C2	-2.19	107.39	110.77
2	W	1	NAG	C3-C4-C5	-2.19	106.33	110.24
3	e	4	MAN	O3-C3-C2	2.19	114.18	109.99
2	f	4	BGC	O5-C1-C2	-2.18	107.40	110.77
2	p	4	BGC	O5-C1-C2	-2.18	107.40	110.77
2	V	5	MAN	O5-C1-C2	2.18	114.14	110.77
2	l	1	NAG	O5-C1-C2	-2.18	107.85	111.29
3	y	3	YZT	O2S6-S6-C6	-2.18	104.35	106.94
2	u	4	BGC	C3-C4-C5	-2.18	106.36	110.24
3	y	4	MAN	O3-C3-C2	2.18	114.16	109.99
3	P	4	MAN	O3-C3-C2	2.17	114.16	109.99
2	R	2	NAG	C3-C4-C5	2.17	114.11	110.24
3	K	3	YZT	O2S6-S6-C6	-2.17	104.36	106.94
2	k	4	BGC	C3-C4-C5	-2.17	106.37	110.24
2	Q	6	MAN	C1-O5-C5	2.16	115.12	112.19
3	K	4	MAN	O3-C3-C2	2.16	114.13	109.99
2	M	2	NAG	C3-C4-C5	2.15	114.08	110.24
2	w	1	NAG	C2-N2-C7	-2.15	119.84	122.90
3	U	3	YZT	O2S6-S6-C6	-2.15	104.38	106.94
3	j	3	YZT	O2S6-S6-C6	-2.15	104.38	106.94
3	t	4	MAN	O3-C3-C2	2.15	114.11	109.99
2	L	4	BGC	C3-C4-C5	-2.15	106.41	110.24
2	f	4	BGC	C3-C4-C5	-2.15	106.41	110.24
2	V	4	BGC	C3-C4-C5	-2.14	106.41	110.24
3	t	3	YZT	O2S6-S6-C6	-2.14	104.39	106.94
3	e	3	YZT	O2S6-S6-C6	-2.14	104.40	106.94
2	z	4	BGC	C3-C4-C5	-2.14	106.43	110.24
2	J	2	NAG	C1-O5-C5	2.13	115.08	112.19
2	a	4	BGC	C3-C4-C5	-2.13	106.44	110.24
2	p	1	NAG	O7-C7-C8	-2.13	118.10	122.06
3	P	3	YZT	O2S6-S6-C6	-2.13	104.41	106.94
2	p	4	BGC	C3-C4-C5	-2.13	106.44	110.24
2	u	6	MAN	C1-C2-C3	2.13	112.28	109.67
2	0	2	NAG	C3-C4-C5	2.13	114.03	110.24
2	l	1	NAG	C2-N2-C7	-2.12	119.88	122.90
2	u	5	MAN	O5-C1-C2	2.12	114.05	110.77
2	R	1	NAG	C3-C4-C5	-2.12	106.45	110.24
3	Z	3	YZT	O2S6-S6-C6	-2.12	104.42	106.94
2	a	5	MAN	O5-C1-C2	2.12	114.04	110.77
2	d	3	YZT	O2S6-S6-C6	-2.11	104.43	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	o	3	YZT	O2S6-S6-C6	-2.11	104.43	106.94
2	Q	4	BGC	C3-C4-C5	-2.11	106.48	110.24
2	L	1	NAG	O5-C1-C2	-2.11	107.96	111.29
2	W	2	NAG	C3-C4-C5	2.10	113.99	110.24
2	M	1	NAG	C3-C4-C5	-2.10	106.49	110.24
2	S	1	NAG	C1-O5-C5	-2.10	109.35	112.19
2	l	2	NAG	C3-C4-C5	2.08	113.95	110.24
2	z	6	MAN	C1-C2-C3	2.08	112.22	109.67
2	g	2	NAG	C3-C4-C5	2.08	113.94	110.24
2	s	2	NAG	C1-O5-C5	2.08	115.00	112.19
2	b	1	NAG	C3-C4-C5	-2.08	106.54	110.24
2	d	4	BGC	C1-C2-C3	2.07	112.22	109.67
2	b	2	NAG	C3-C4-C5	2.07	113.94	110.24
2	S	4	BGC	O4-C4-C3	-2.07	105.57	110.35
2	h	4	BGC	O4-C4-C3	-2.07	105.57	110.35
2	f	5	MAN	O5-C1-C2	2.06	113.96	110.77
2	l	4	BGC	O4-C4-C3	-2.06	105.58	110.35
2	n	2	NAG	C1-O5-C5	2.06	114.99	112.19
2	T	4	BGC	C1-C2-C3	2.06	112.20	109.67
2	V	6	MAN	C1-C2-C3	2.06	112.20	109.67
2	v	2	NAG	C3-C4-C5	2.06	113.91	110.24
2	z	5	MAN	O5-C1-C2	2.06	113.95	110.77
2	X	4	BGC	O4-C4-C3	-2.06	105.59	110.35
2	O	4	BGC	C1-C2-C3	2.05	112.19	109.67
2	N	4	BGC	O4-C4-C3	-2.05	105.62	110.35
2	w	4	BGC	O4-C4-C3	-2.04	105.62	110.35
2	q	2	NAG	C3-C4-C5	2.04	113.88	110.24
2	r	4	BGC	O4-C4-C3	-2.04	105.64	110.35
2	w	2	NAG	O3-C3-C4	-2.03	105.66	110.35
2	N	1	NAG	C1-O5-C5	-2.03	109.45	112.19
2	m	4	BGC	O4-C4-C3	-2.03	105.67	110.35
2	i	4	BGC	C1-C2-C3	2.02	112.16	109.67
2	l	2	NAG	O3-C3-C4	-2.02	105.67	110.35
2	r	2	NAG	O3-C3-C4	-2.02	105.68	110.35
2	d	2	NAG	C1-O5-C5	2.02	114.93	112.19
2	a	4	BGC	O6-C6-C5	-2.02	104.37	111.29
2	c	2	NAG	O3-C3-C4	-2.01	105.69	110.35
2	u	4	BGC	O6-C6-C5	-2.01	104.39	111.29
2	s	4	BGC	C1-C2-C3	2.01	112.14	109.67
2	k	2	NAG	C3-C4-C5	2.01	113.82	110.24
2	v	1	NAG	C3-C4-C5	-2.01	106.66	110.24
2	c	4	BGC	O4-C4-C3	-2.01	105.71	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	2	NAG	O3-C3-C4	-2.01	105.71	110.35
2	Q	4	BGC	O6-C6-C5	-2.00	104.41	111.29
2	f	4	BGC	O6-C6-C5	-2.00	104.42	111.29
2	p	4	BGC	O6-C6-C5	-2.00	104.42	111.29

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C3-C2-N2-C7
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	U	2	NAG	C3-C2-N2-C7
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	Z	2	NAG	C3-C2-N2-C7
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
3	e	1	NAG	C8-C7-N2-C2
3	e	1	NAG	O7-C7-N2-C2
3	e	2	NAG	C3-C2-N2-C7
3	e	2	NAG	C8-C7-N2-C2
3	e	2	NAG	O7-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2
3	j	2	NAG	C3-C2-N2-C7
3	j	2	NAG	C8-C7-N2-C2
3	j	2	NAG	O7-C7-N2-C2
3	o	1	NAG	C8-C7-N2-C2
3	o	1	NAG	O7-C7-N2-C2
3	o	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	o	2	NAG	C8-C7-N2-C2
3	o	2	NAG	O7-C7-N2-C2
3	t	1	NAG	C8-C7-N2-C2
3	t	1	NAG	O7-C7-N2-C2
3	t	2	NAG	C3-C2-N2-C7
3	t	2	NAG	C8-C7-N2-C2
3	t	2	NAG	O7-C7-N2-C2
3	y	1	NAG	C8-C7-N2-C2
3	y	1	NAG	O7-C7-N2-C2
3	y	2	NAG	C3-C2-N2-C7
3	y	2	NAG	C8-C7-N2-C2
3	y	2	NAG	O7-C7-N2-C2
2	R	1	NAG	C8-C7-N2-C2
2	W	1	NAG	C8-C7-N2-C2
2	b	1	NAG	C8-C7-N2-C2
2	g	1	NAG	C8-C7-N2-C2
2	q	1	NAG	C8-C7-N2-C2
2	v	1	NAG	C8-C7-N2-C2
2	0	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6
2	w	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C8-C7-N2-C2
2	l	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
2	m	1	NAG	O5-C5-C6-O6
2	s	1	NAG	O5-C5-C6-O6
2	x	1	NAG	O5-C5-C6-O6
2	1	1	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	i	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	x	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6
2	n	1	NAG	C4-C5-C6-O6
2	r	1	NAG	C4-C5-C6-O6
2	s	1	NAG	C4-C5-C6-O6
2	w	1	NAG	C4-C5-C6-O6
2	l	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O7-C7-N2-C2
2	R	1	NAG	O7-C7-N2-C2
2	W	1	NAG	O7-C7-N2-C2
2	b	1	NAG	O7-C7-N2-C2
2	g	1	NAG	O7-C7-N2-C2
2	l	1	NAG	O7-C7-N2-C2
2	q	1	NAG	O7-C7-N2-C2
2	v	1	NAG	O7-C7-N2-C2
2	0	1	NAG	O7-C7-N2-C2
2	S	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	r	2	NAG	O5-C5-C6-O6
2	w	2	NAG	O5-C5-C6-O6
2	l	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
2	s	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	n	2	NAG	O5-C5-C6-O6
2	x	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	d	2	NAG	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
2	p	1	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	z	1	NAG	O5-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	r	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	w	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	l	2	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	u	1	NAG	O5-C5-C6-O6
2	s	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	x	2	NAG	C4-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	M	3	YZT	C5-C6-S6-O1S6
2	R	3	YZT	C5-C6-S6-O1S6
2	W	3	YZT	C5-C6-S6-O1S6
2	b	3	YZT	C5-C6-S6-O1S6
2	g	3	YZT	C5-C6-S6-O1S6
2	l	3	YZT	C5-C6-S6-O1S6
2	q	3	YZT	C5-C6-S6-O1S6
2	v	3	YZT	C5-C6-S6-O1S6
2	0	3	YZT	C5-C6-S6-O1S6
2	O	2	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6

All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	k	5	MAN	C1-C2-C3-C4-C5-O5
2	p	5	MAN	C1-C2-C3-C4-C5-O5

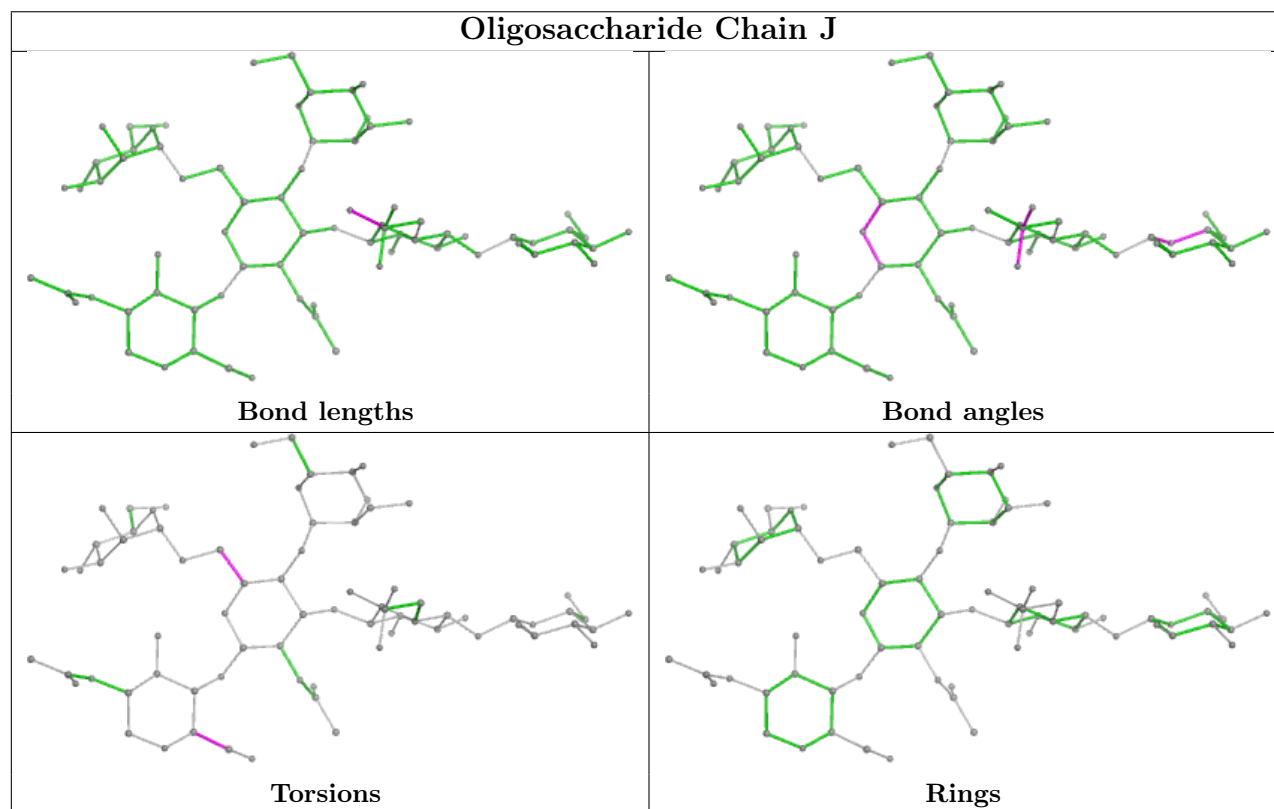
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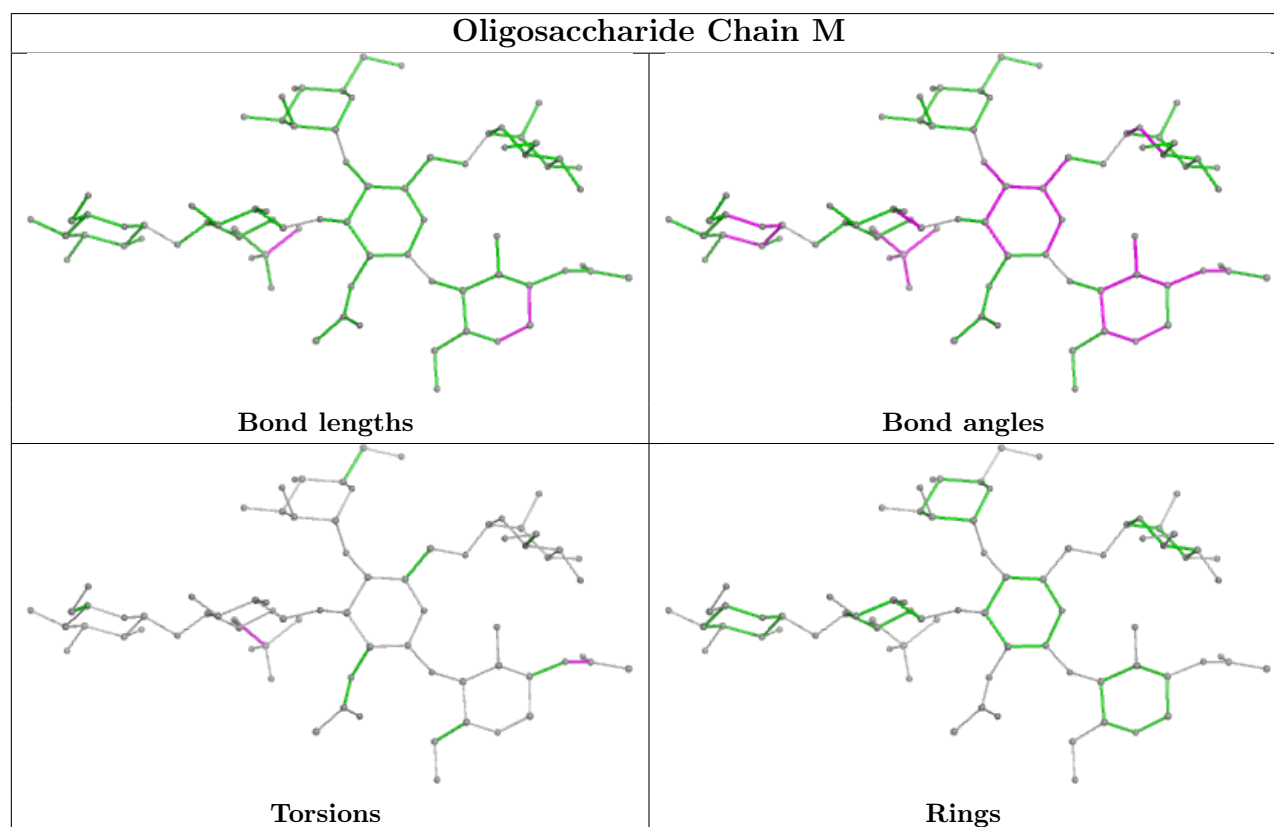
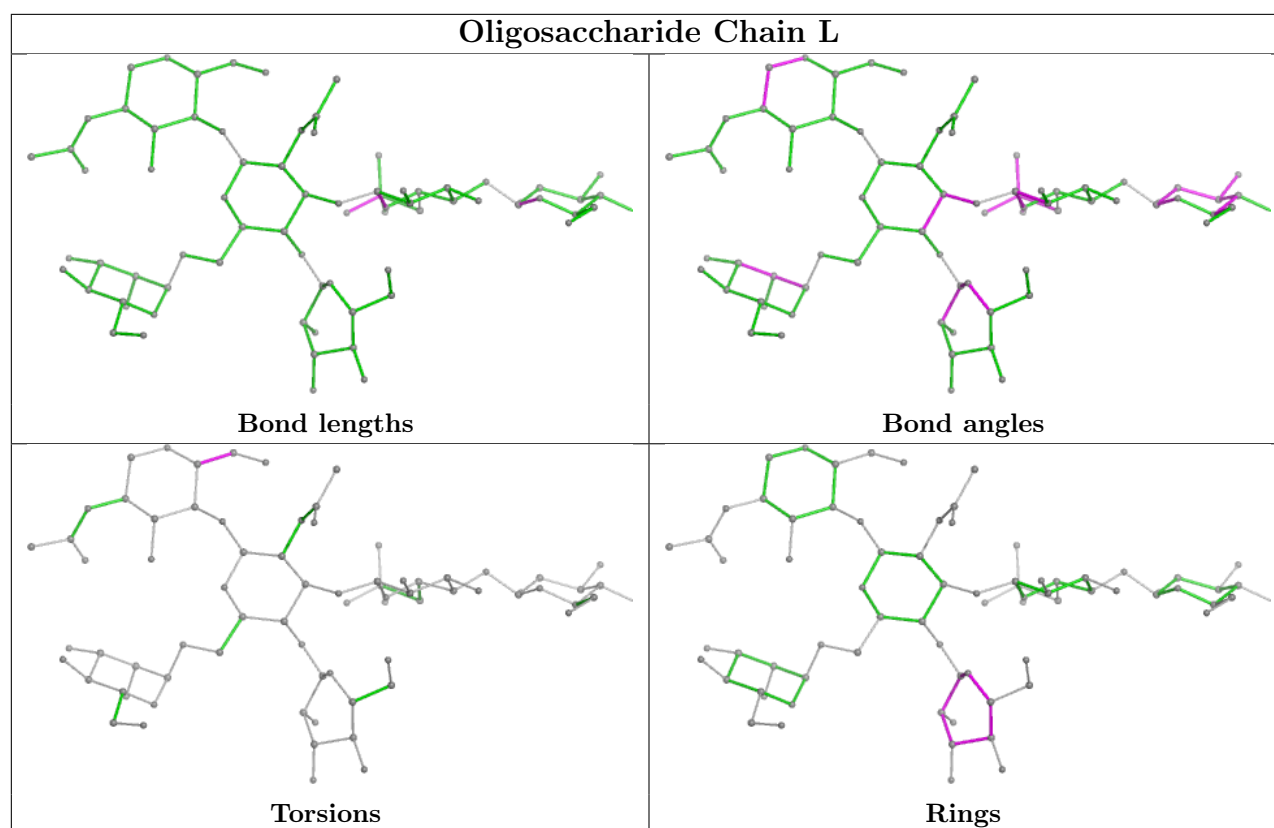
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Mol	Chain	Res	Type	Atoms
2	Q	5	MAN	C1-C2-C3-C4-C5-O5
2	L	5	MAN	C1-C2-C3-C4-C5-O5
2	f	5	MAN	C1-C2-C3-C4-C5-O5
2	u	5	MAN	C1-C2-C3-C4-C5-O5
2	z	5	MAN	C1-C2-C3-C4-C5-O5
2	a	5	MAN	C1-C2-C3-C4-C5-O5
2	V	5	MAN	C1-C2-C3-C4-C5-O5

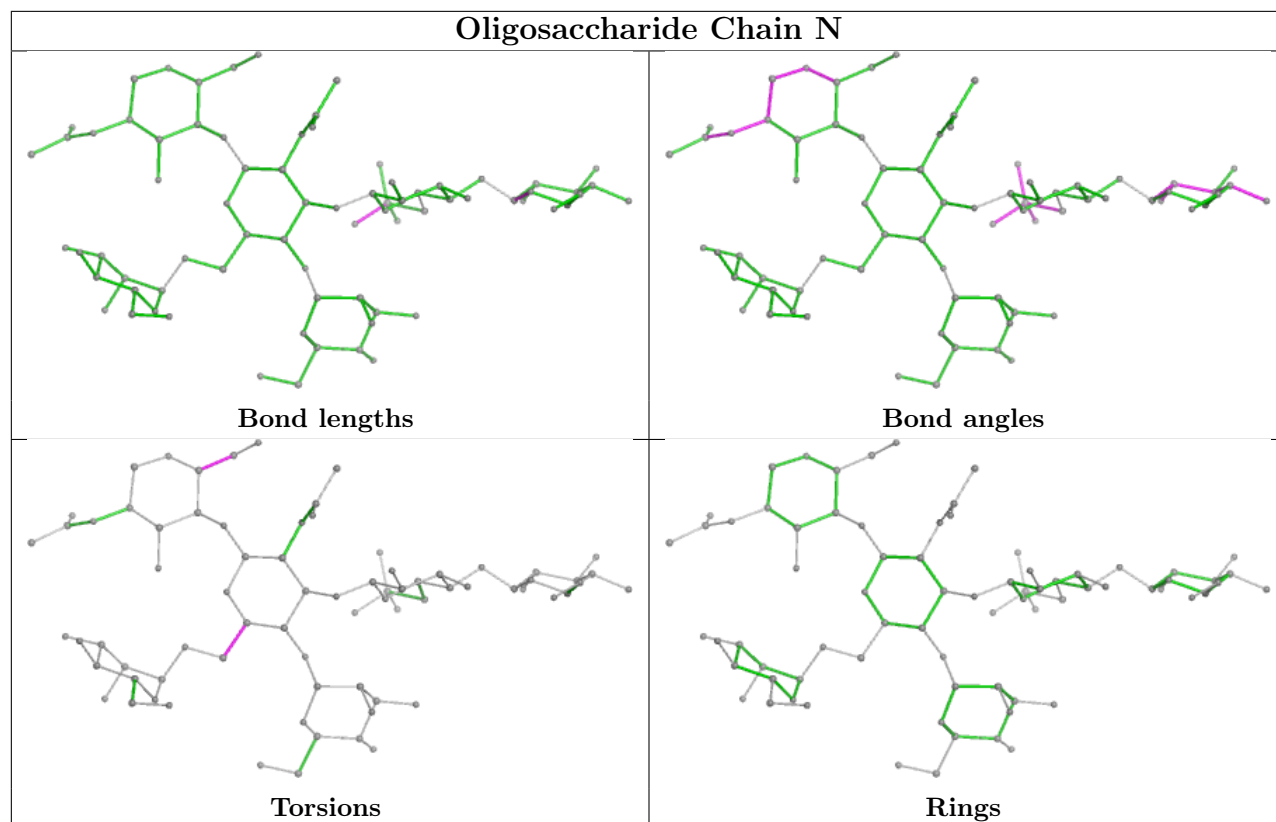
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

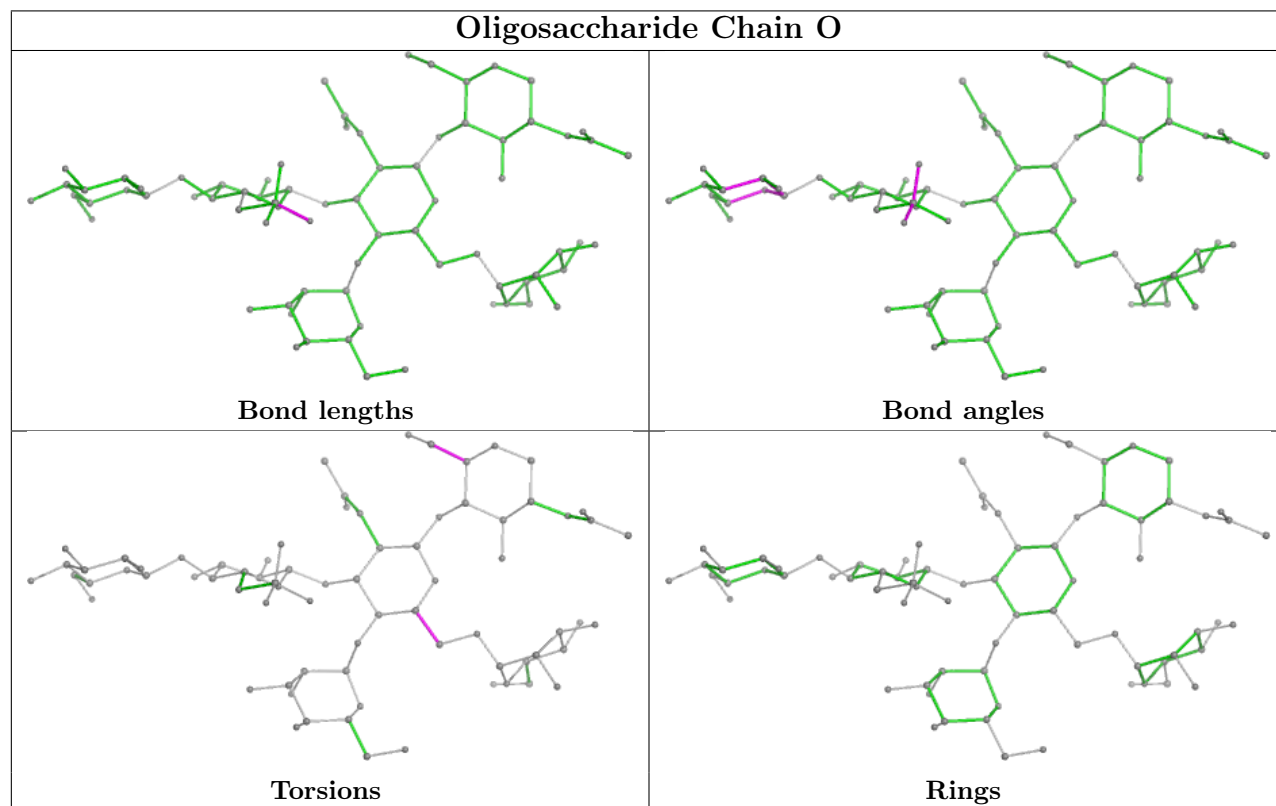


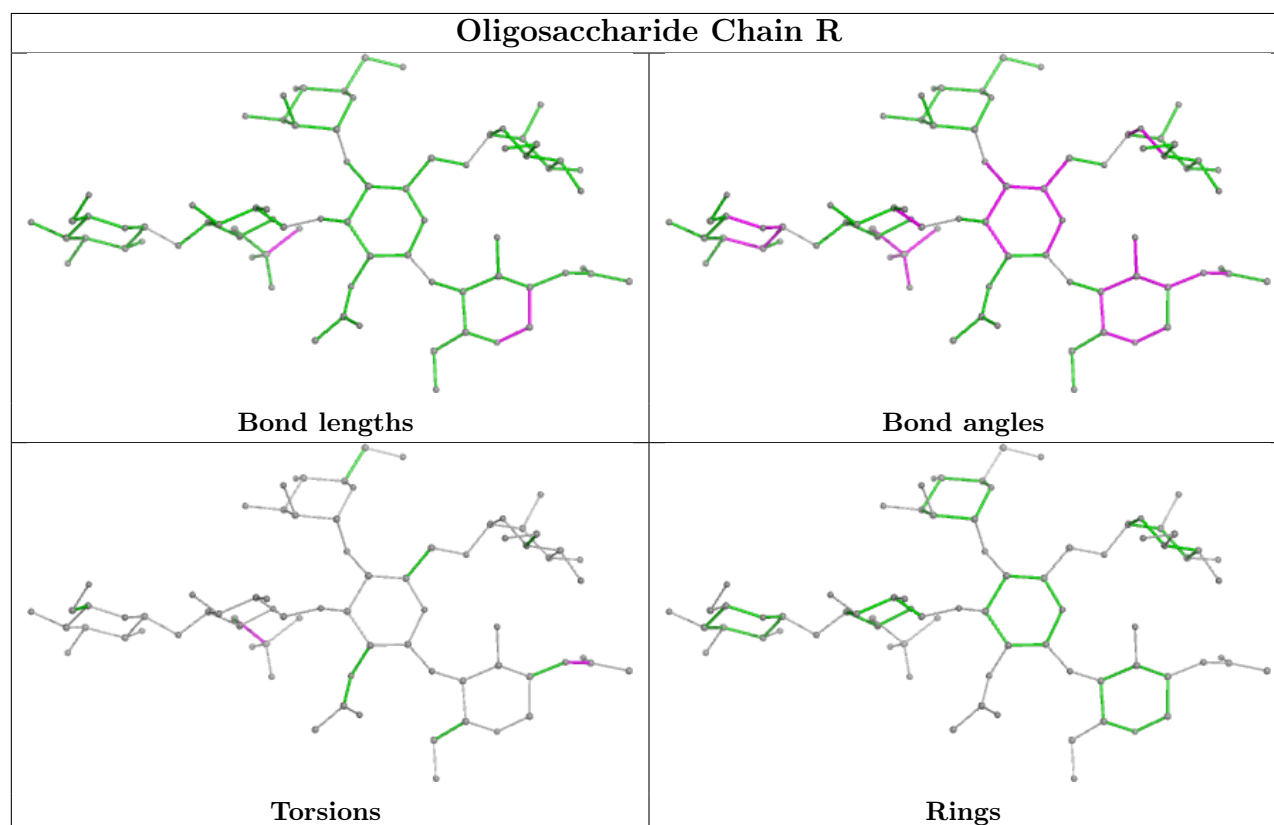
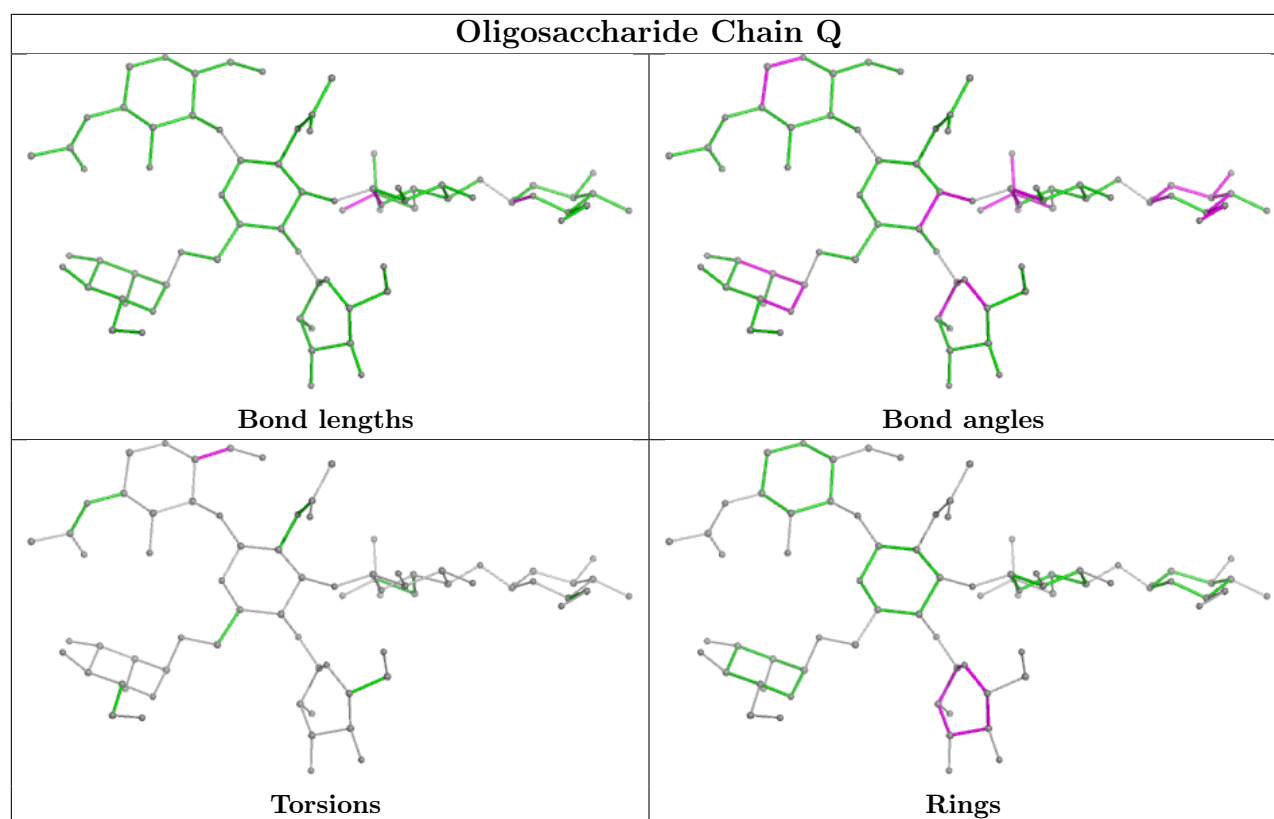


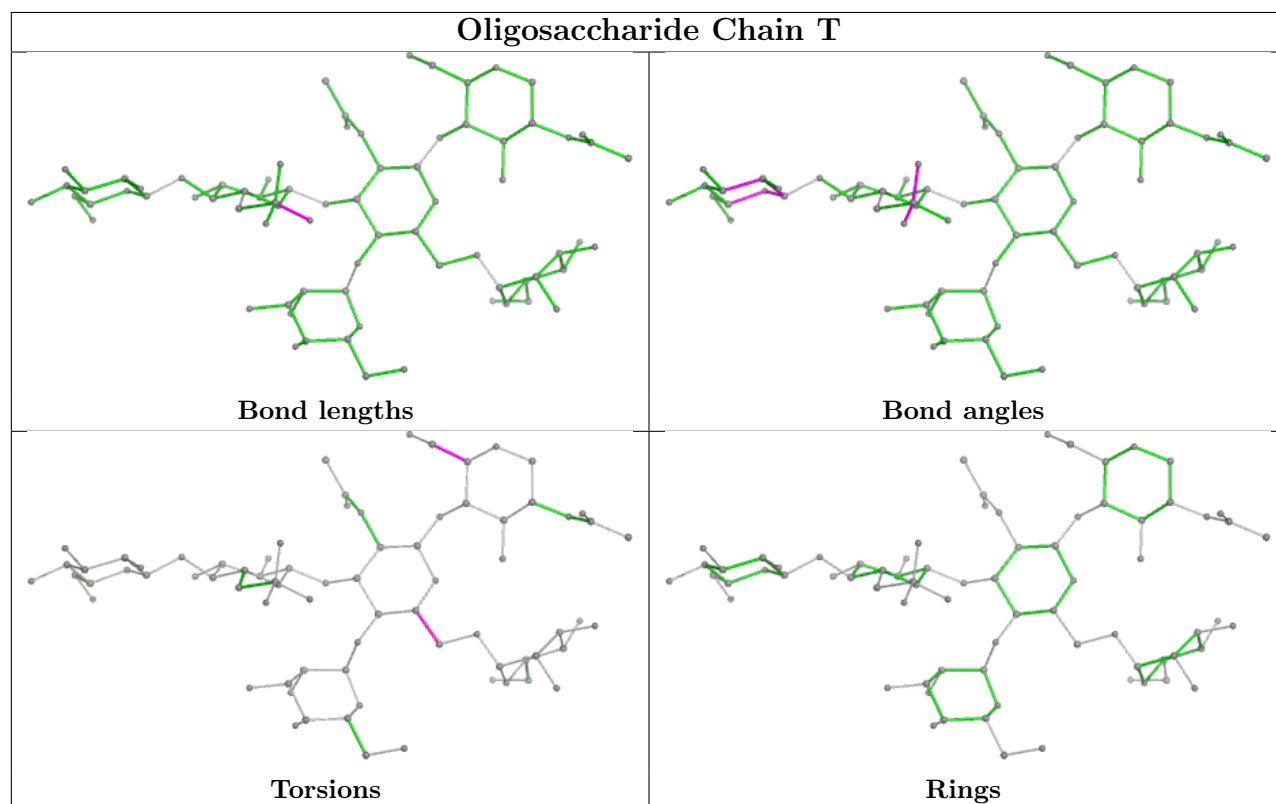
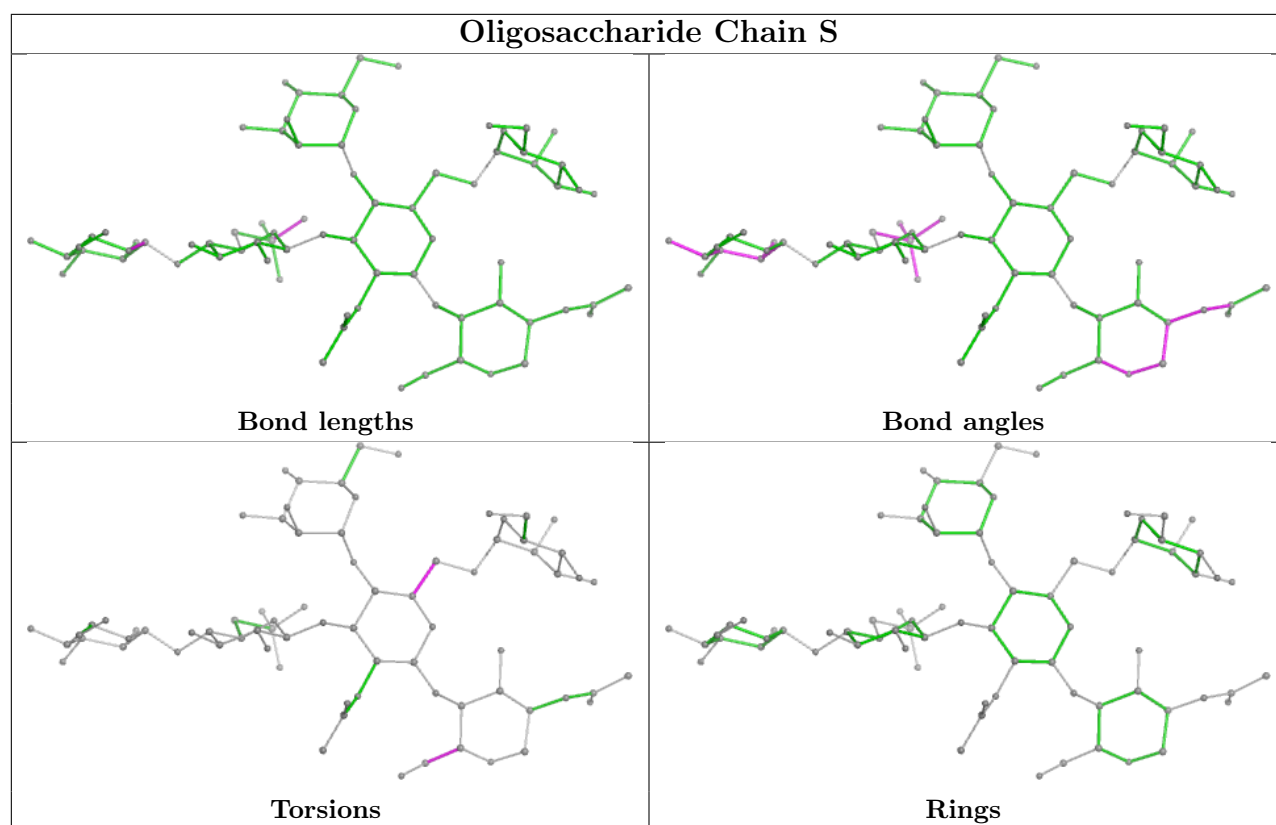
Oligosaccharide Chain N

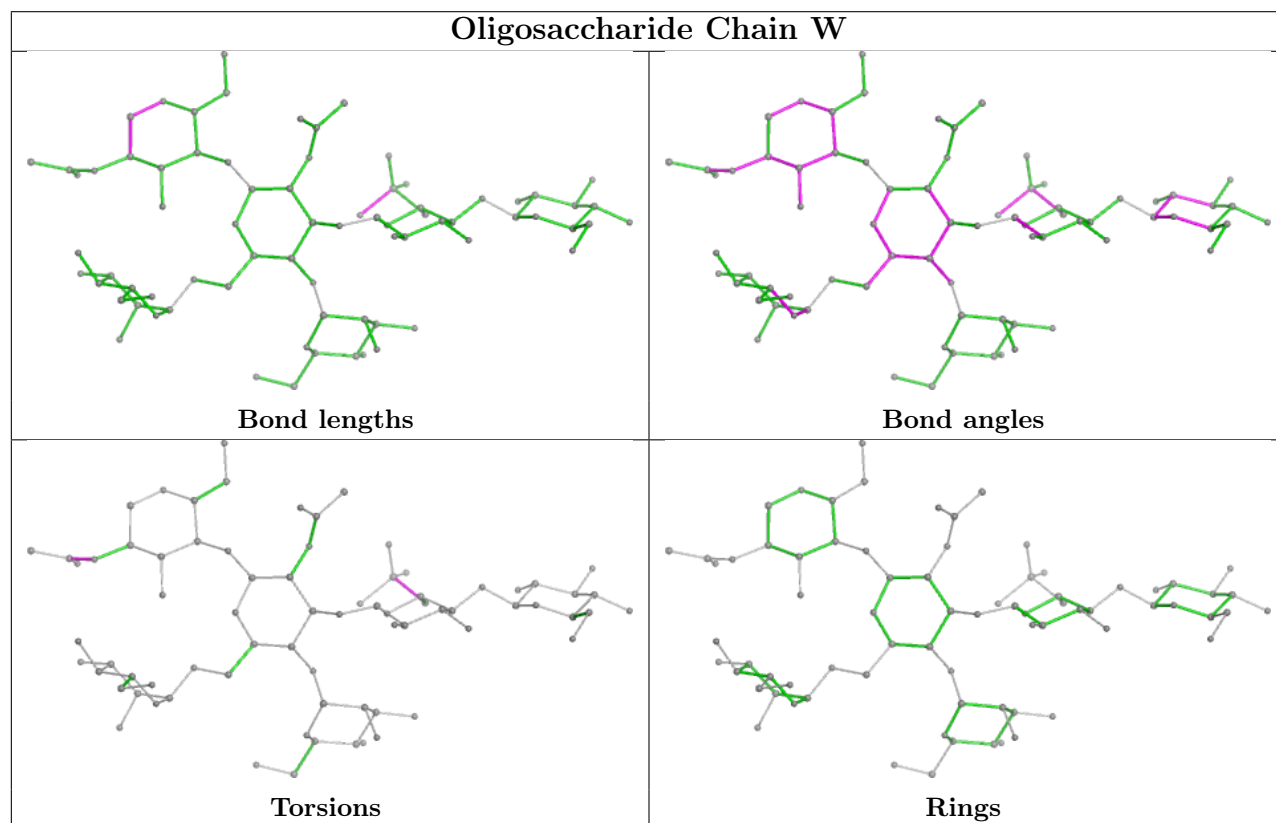
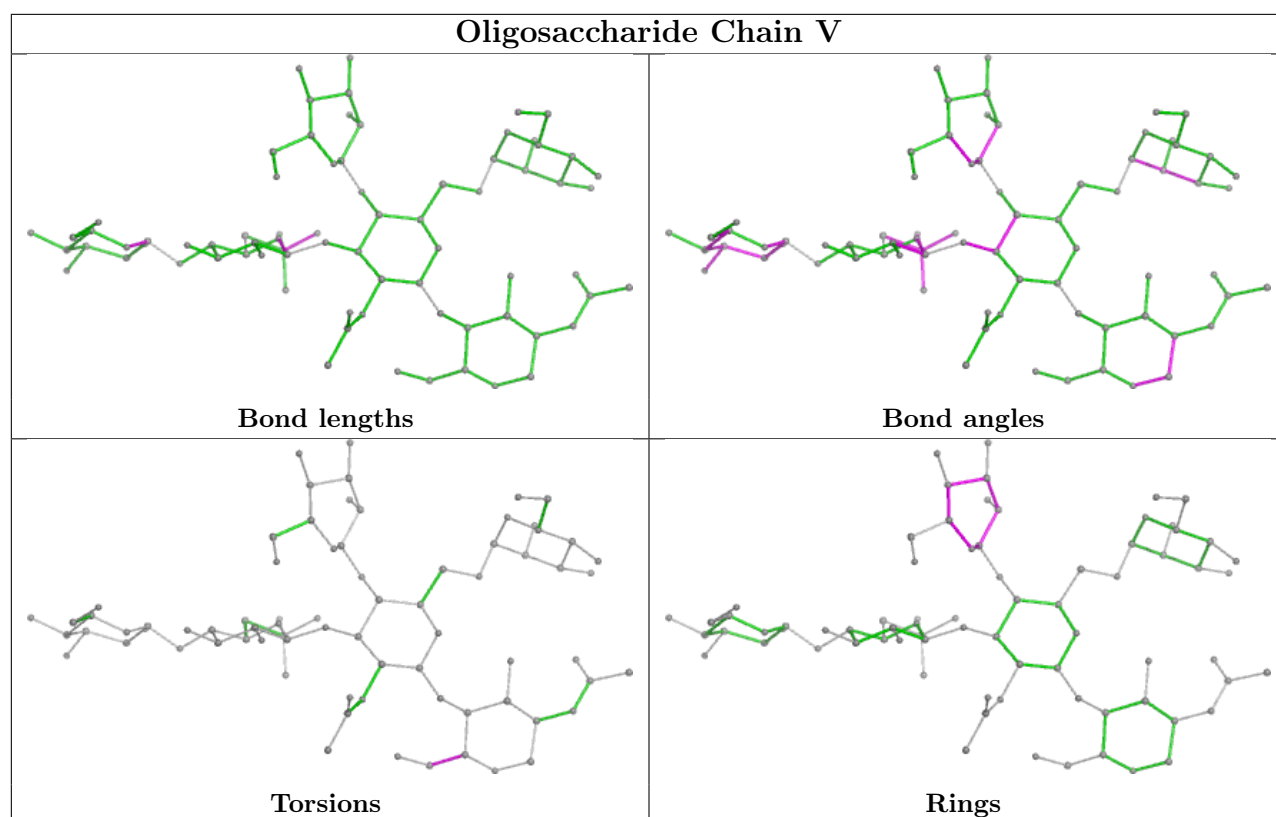


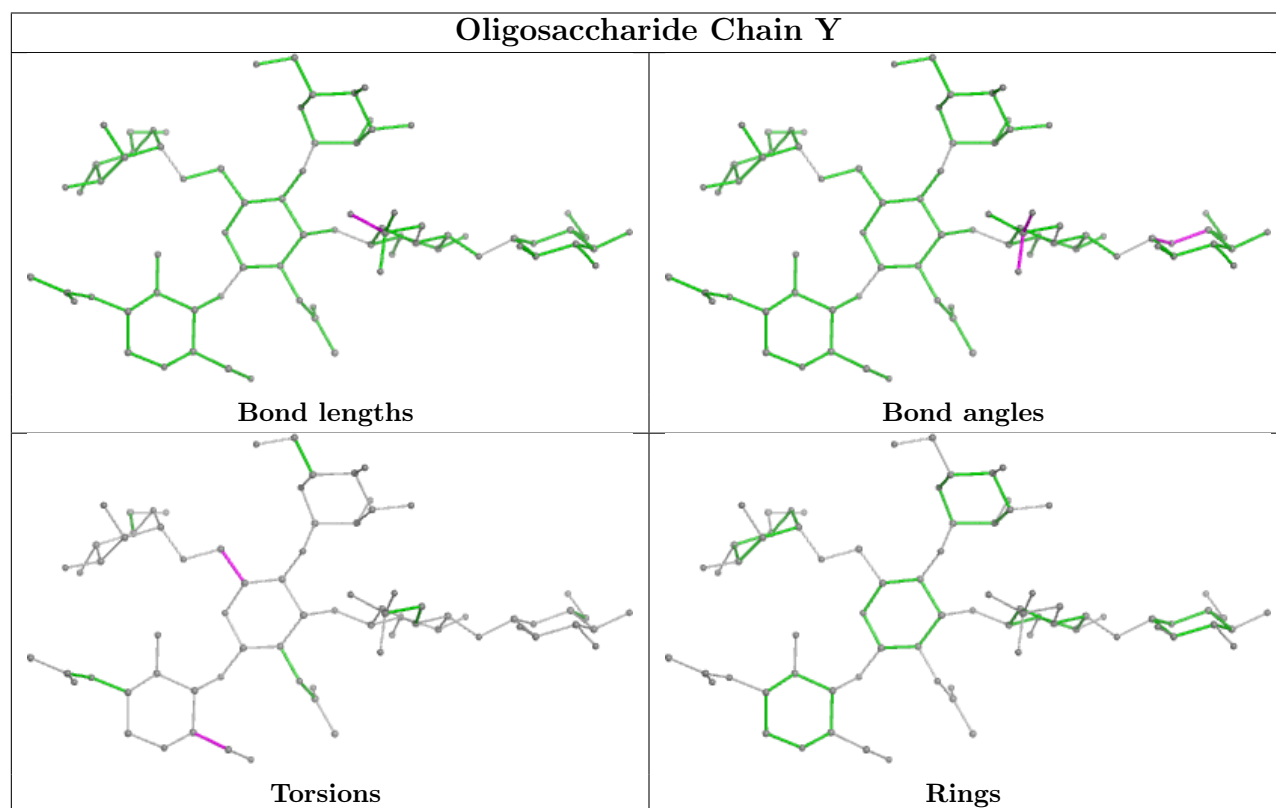
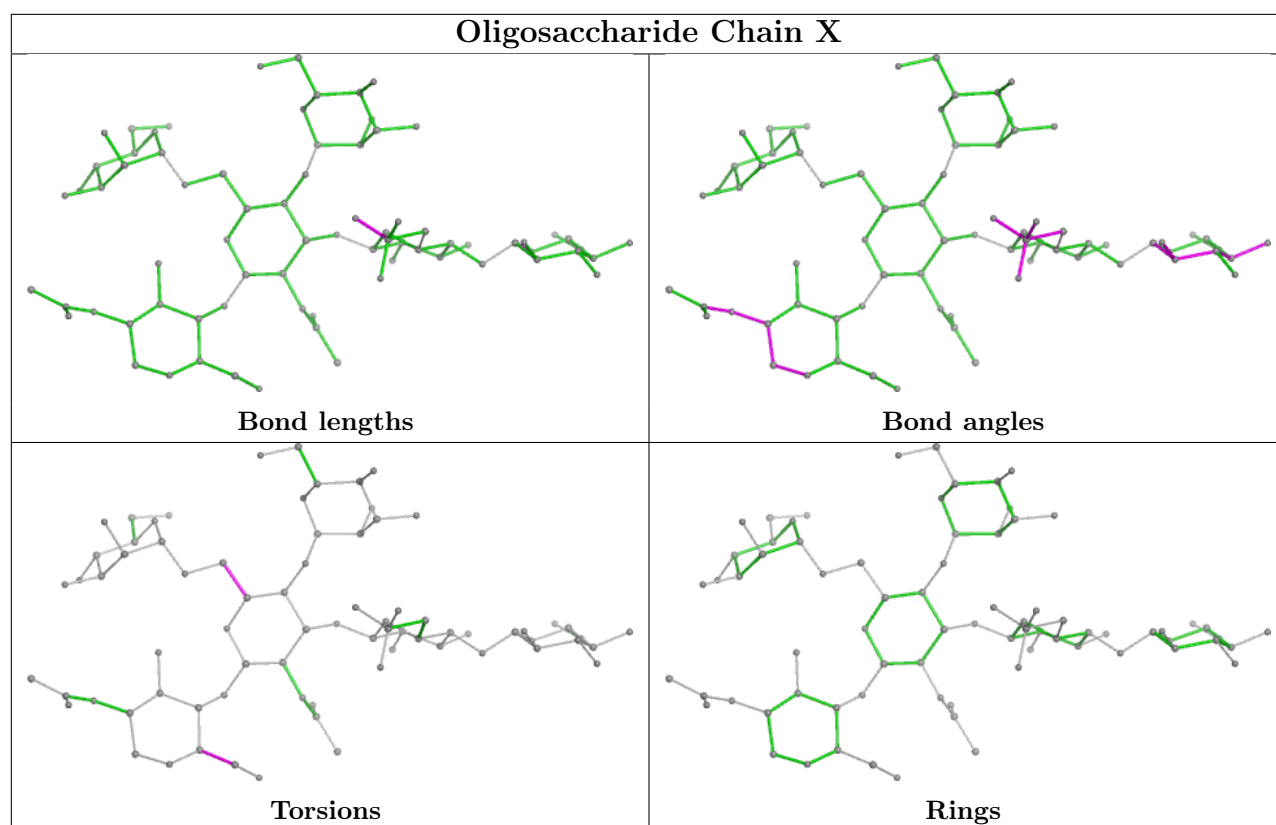
Oligosaccharide Chain O

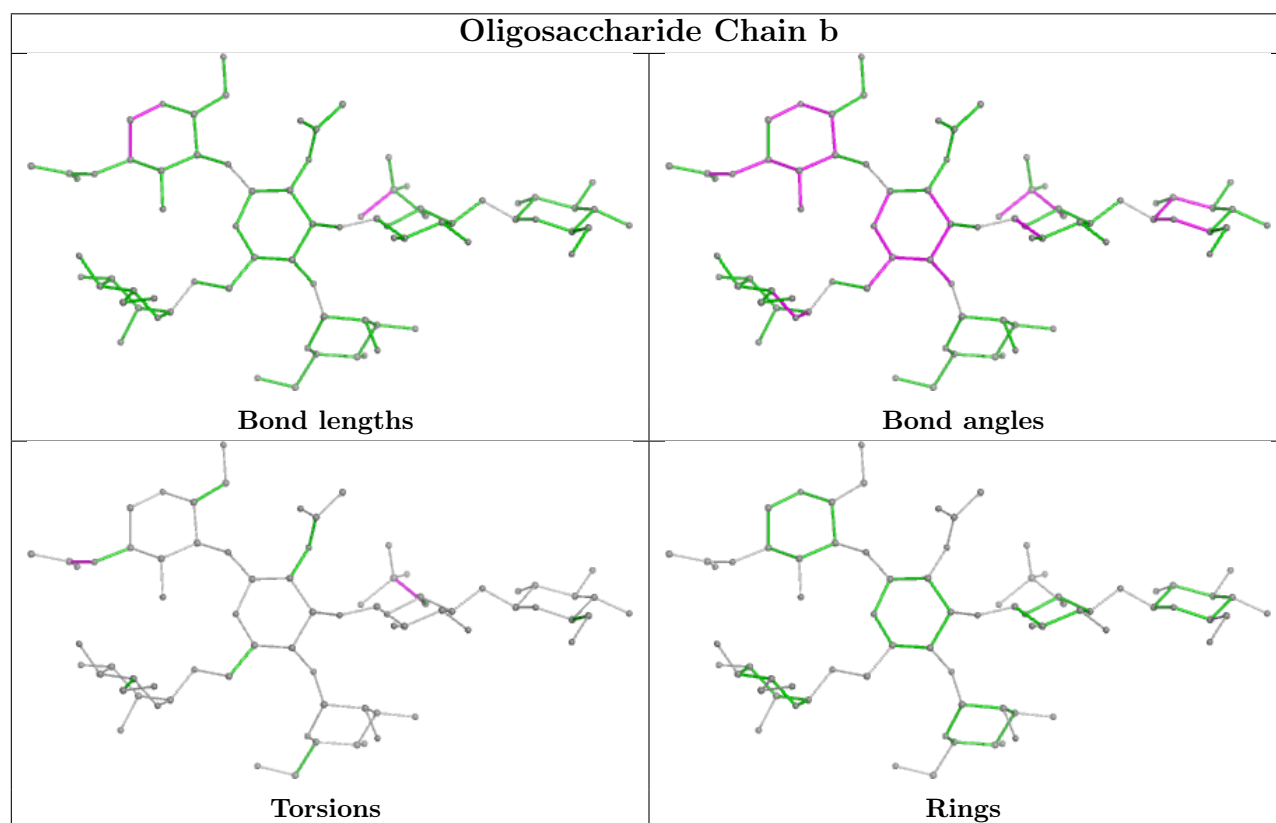
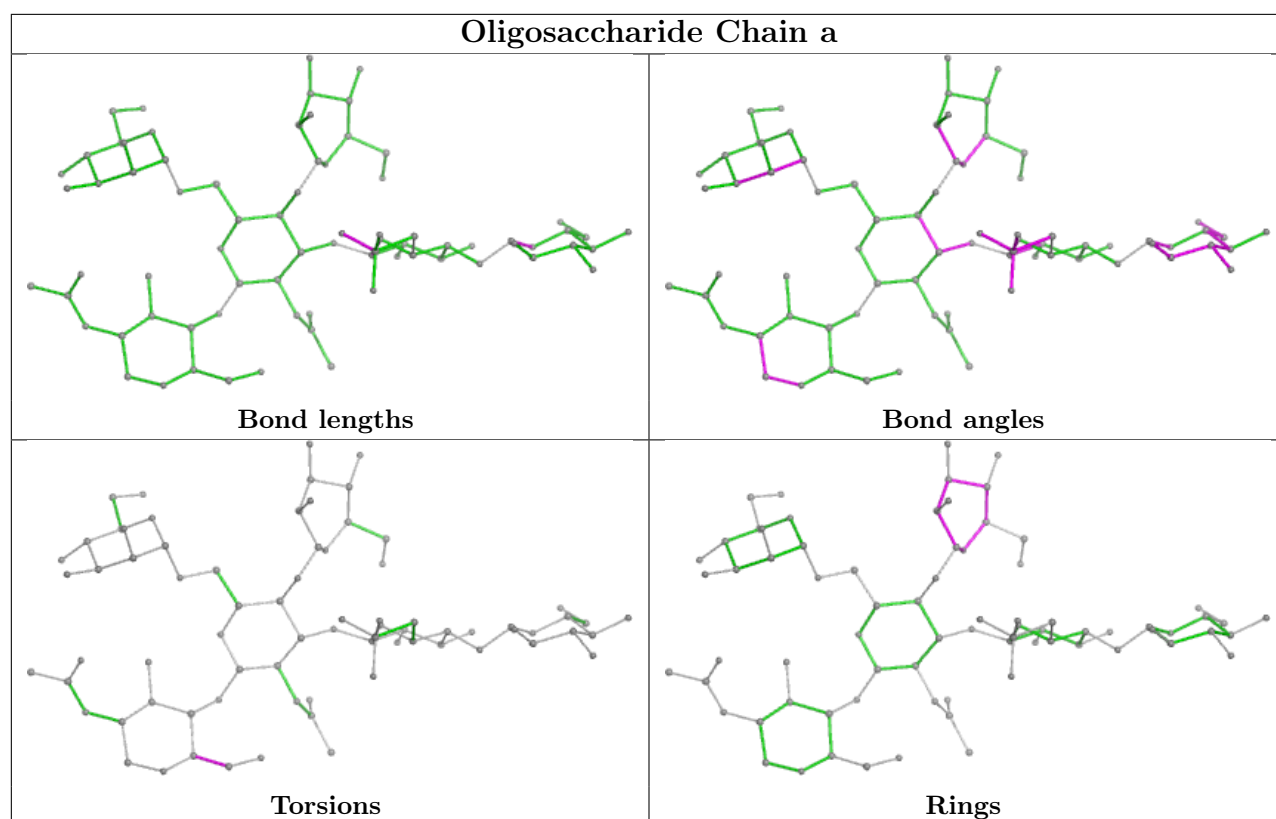


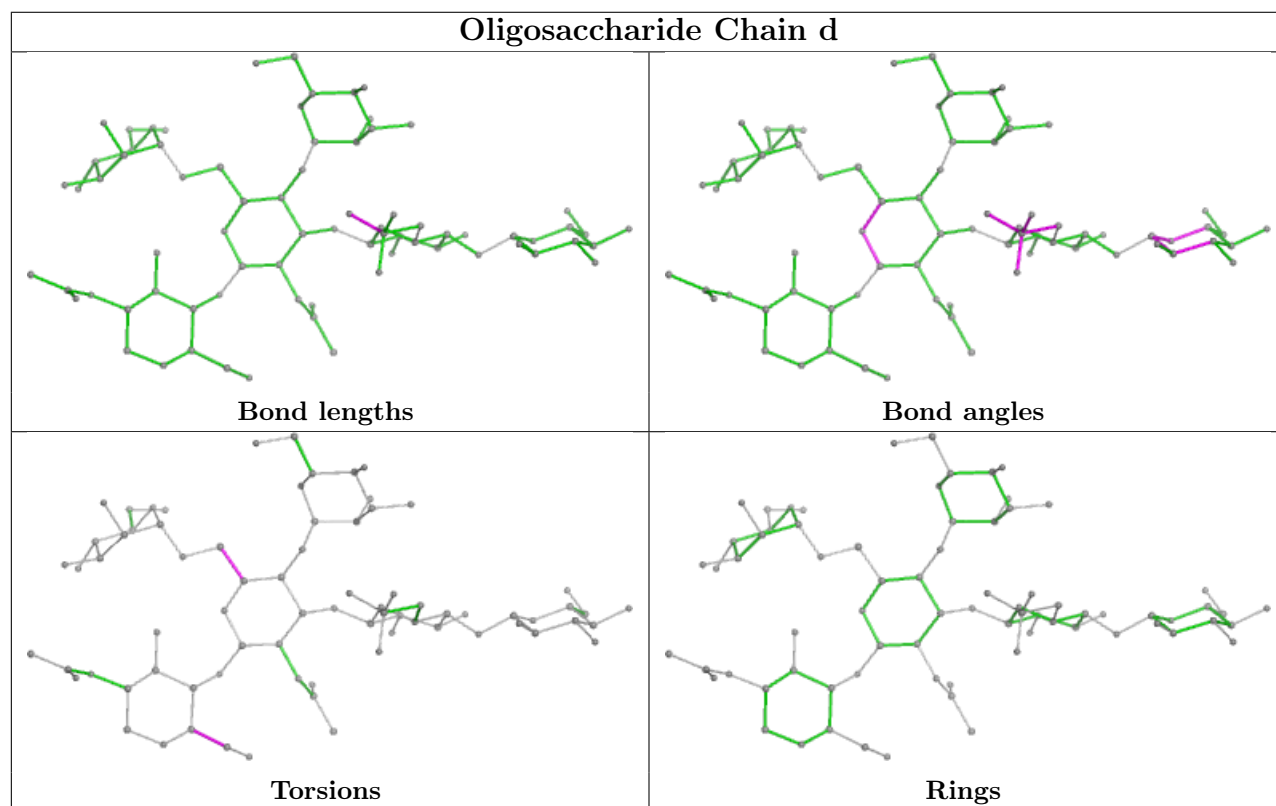
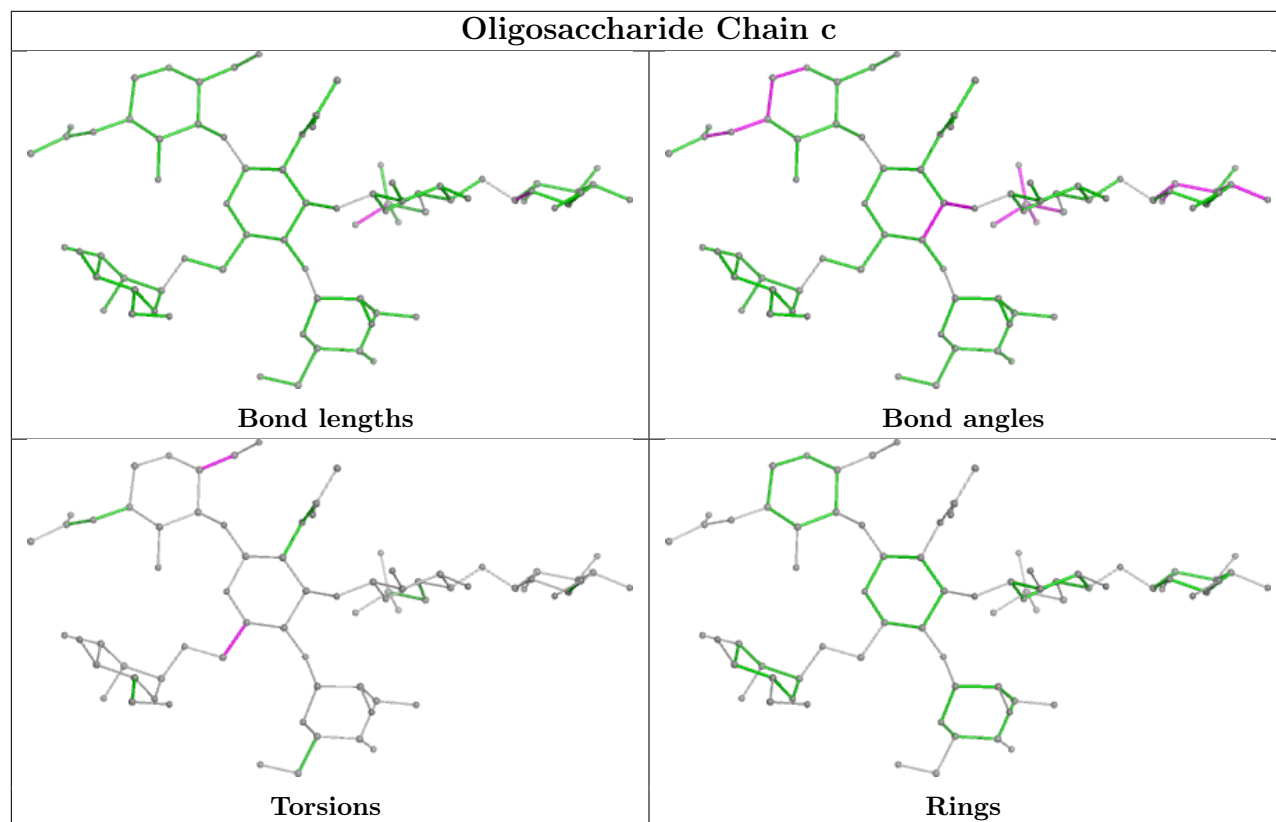


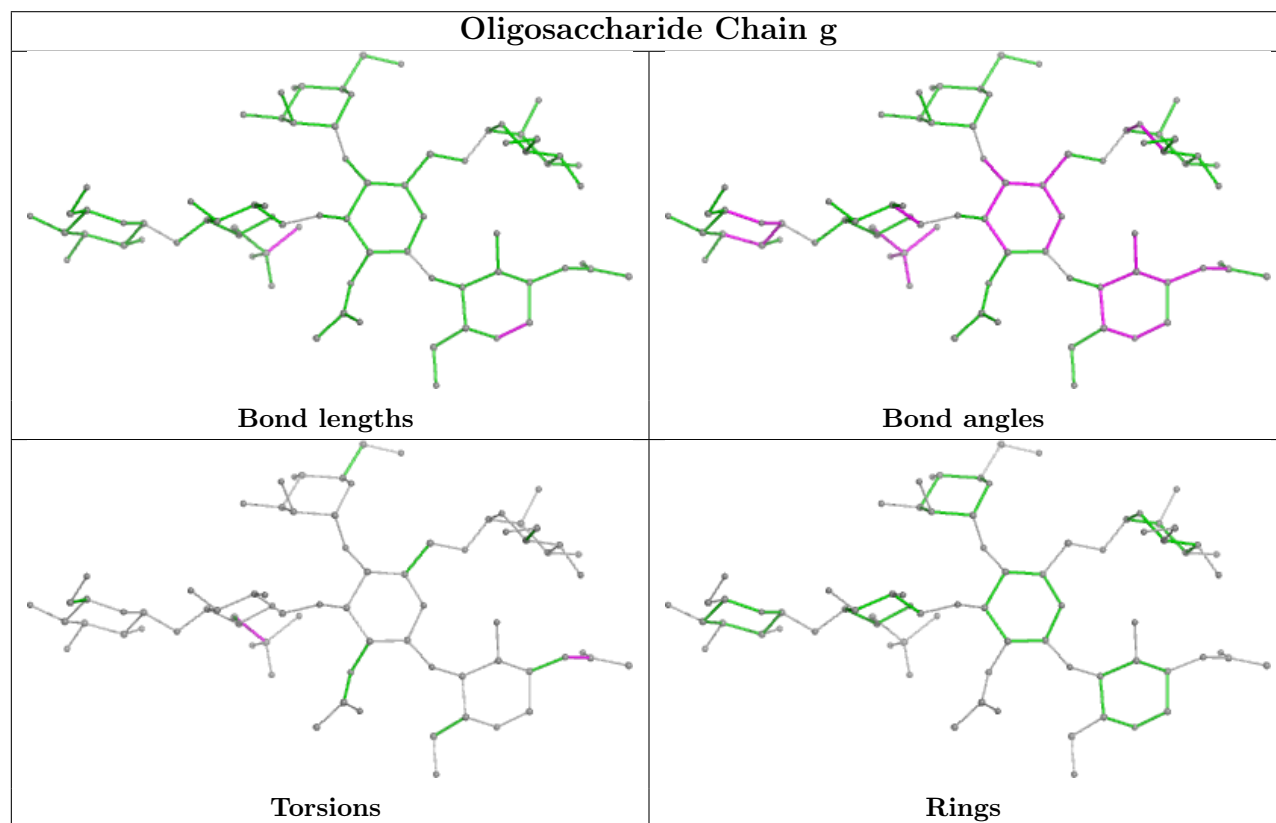
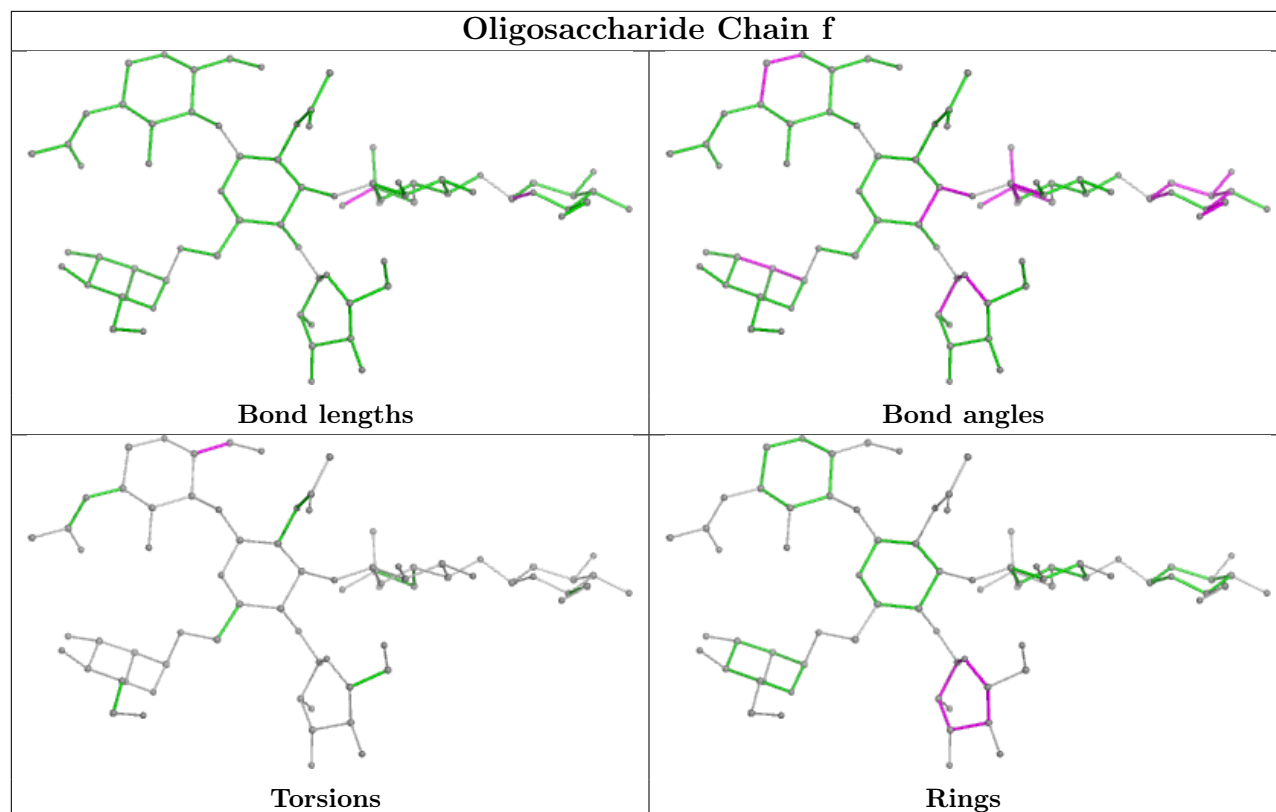


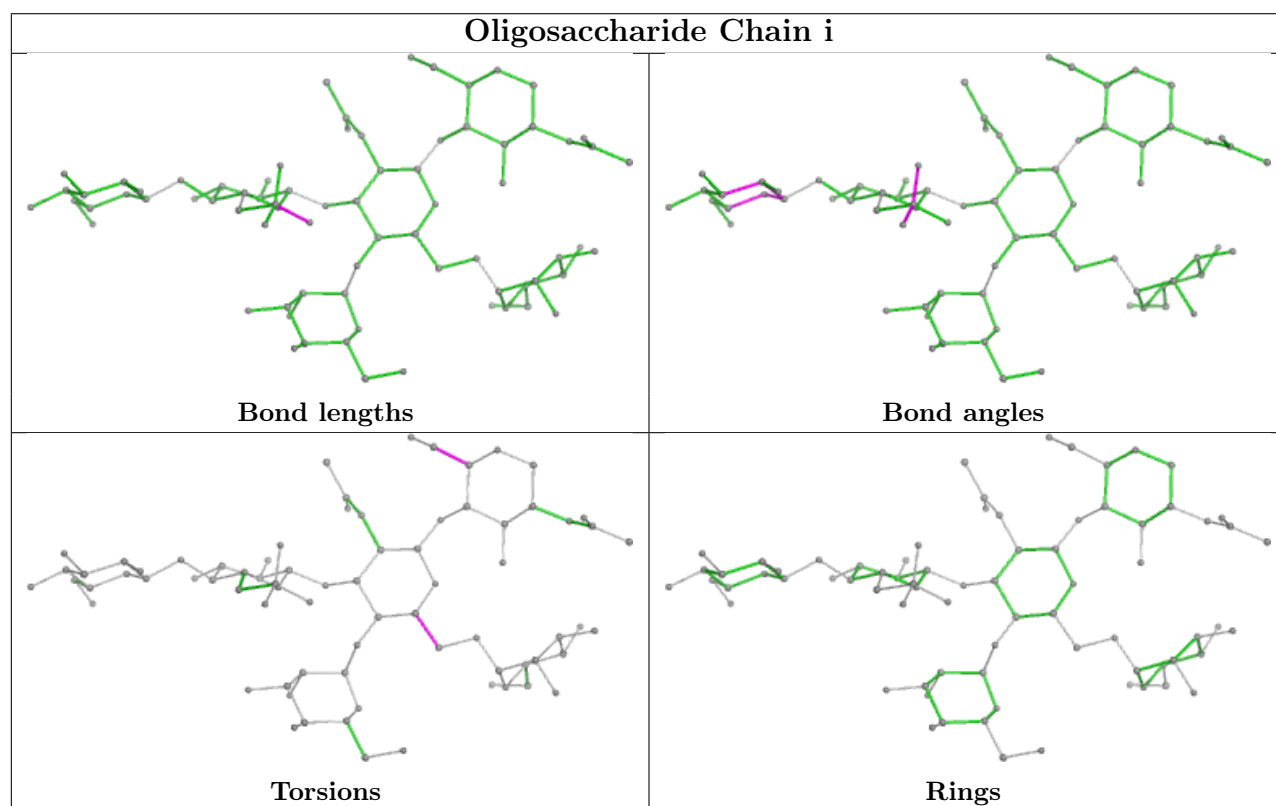
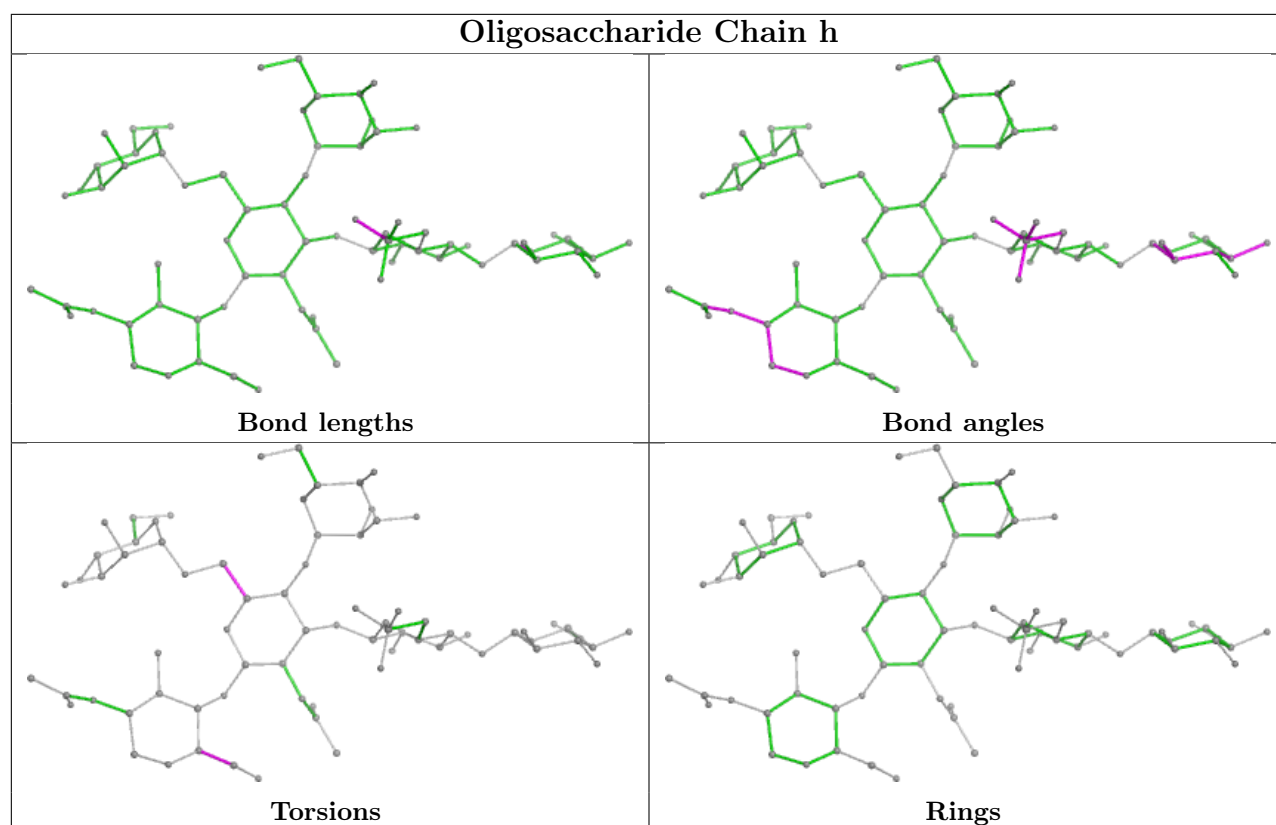


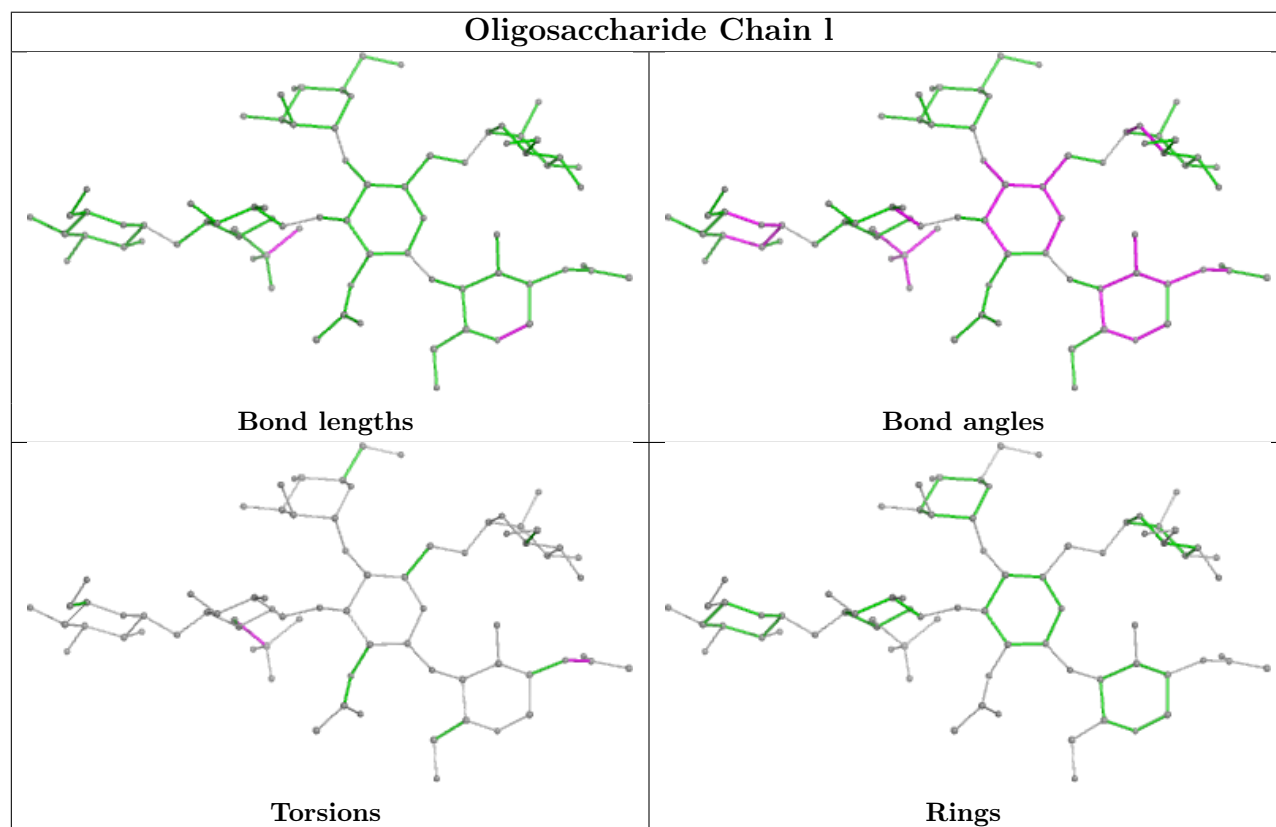
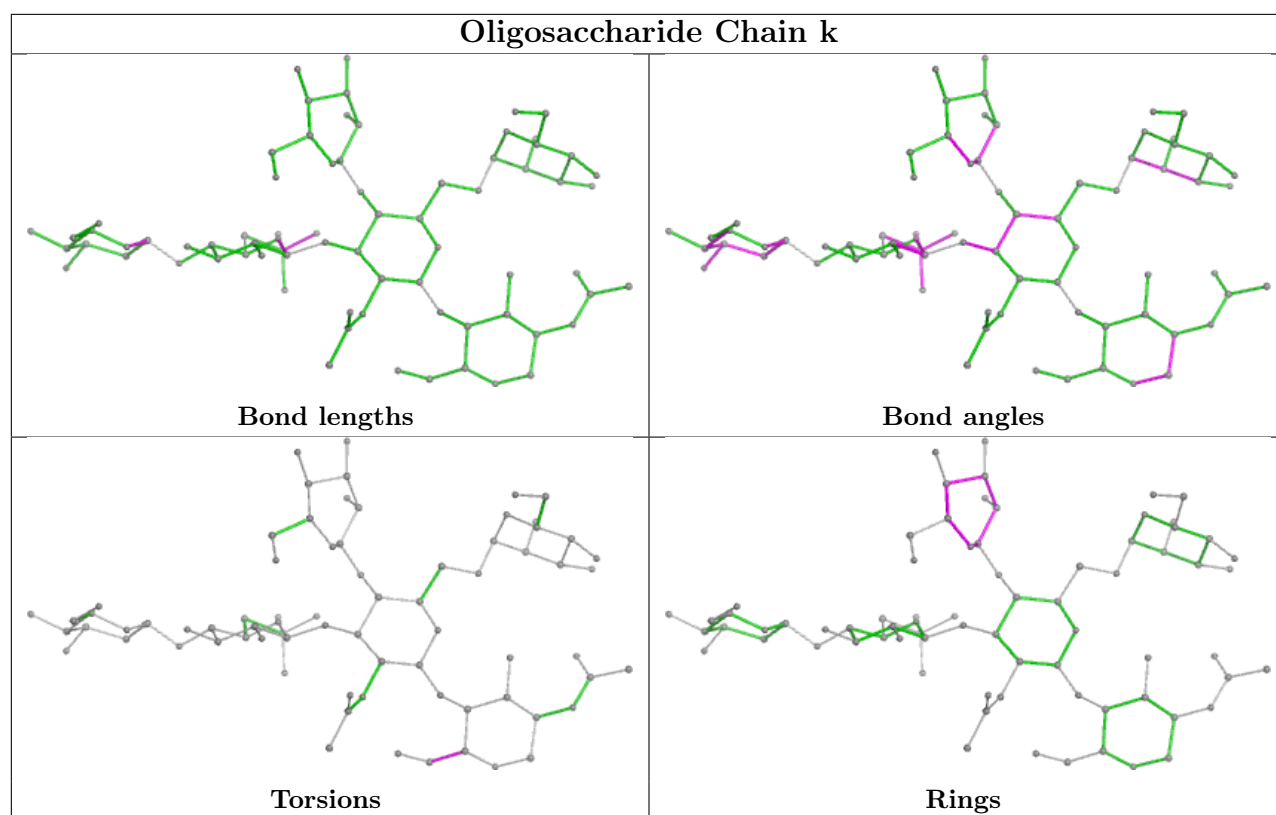


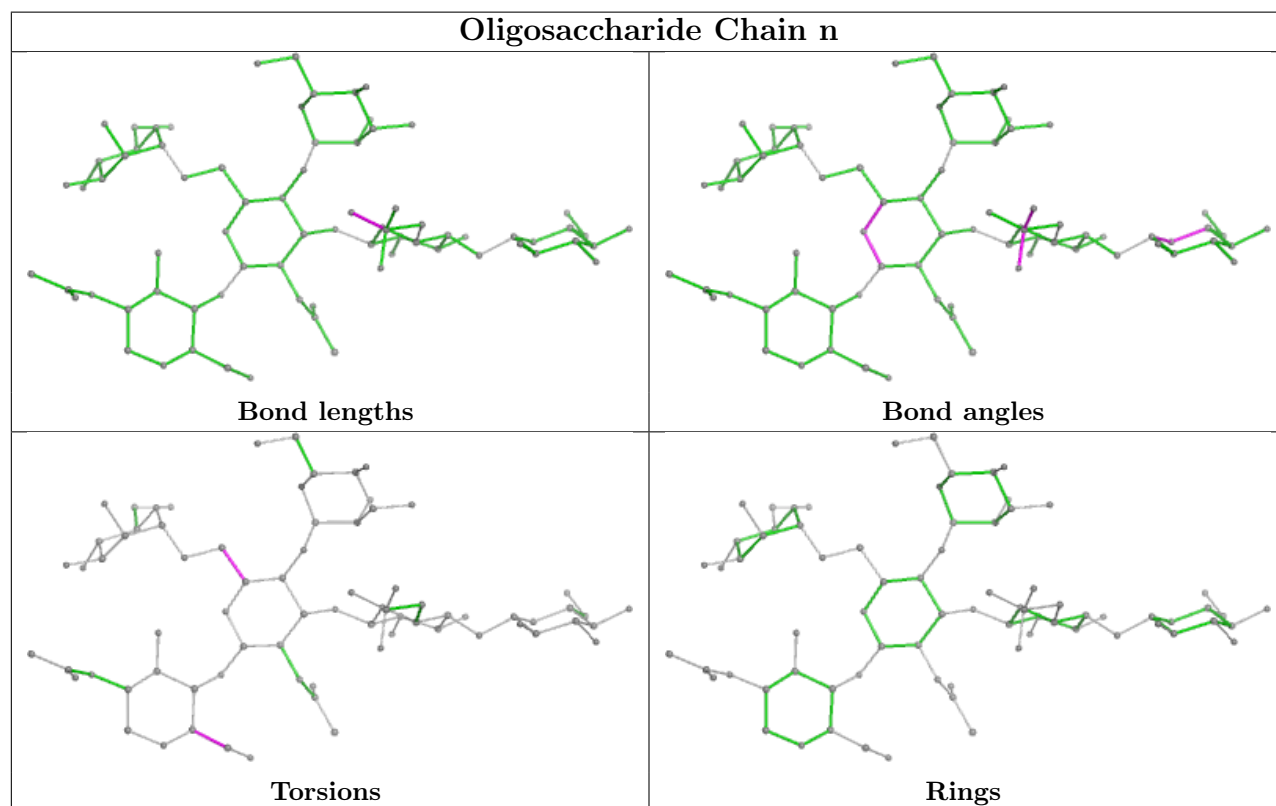
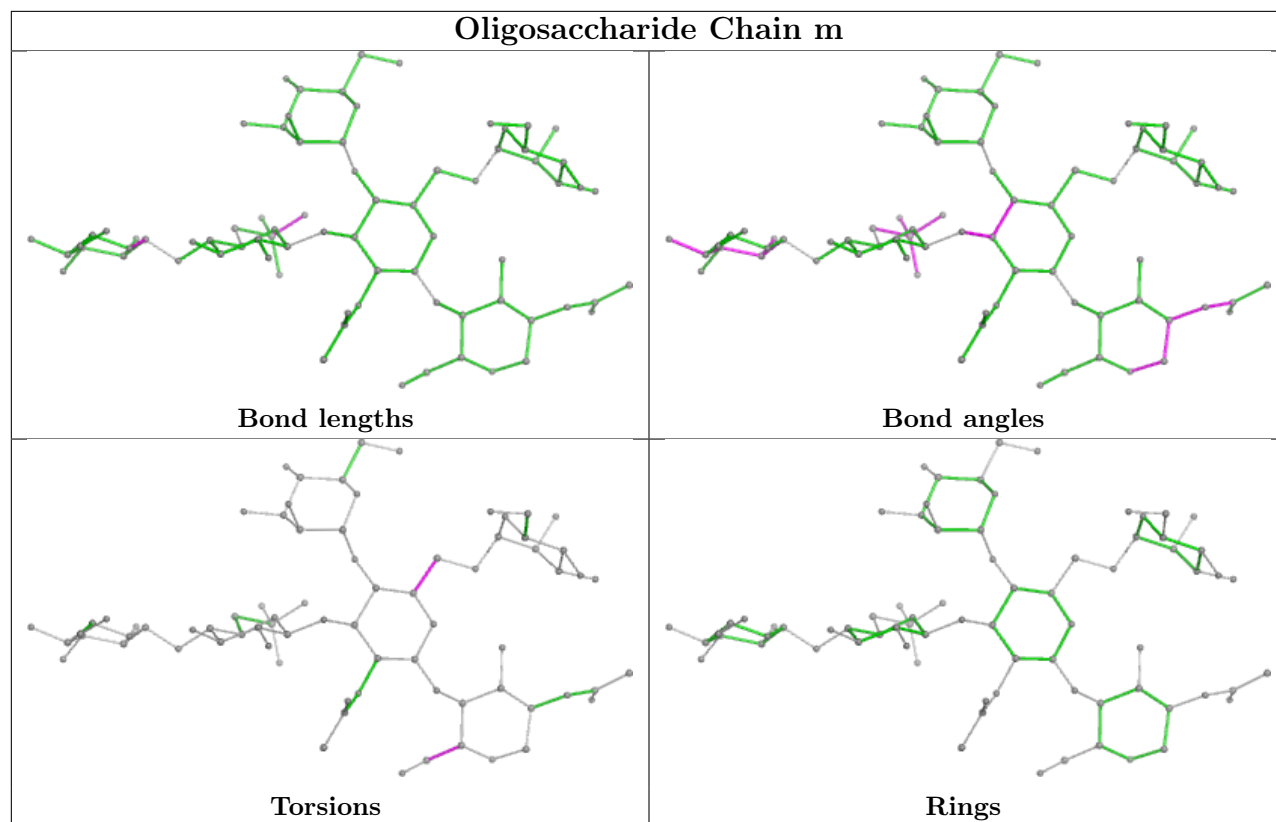


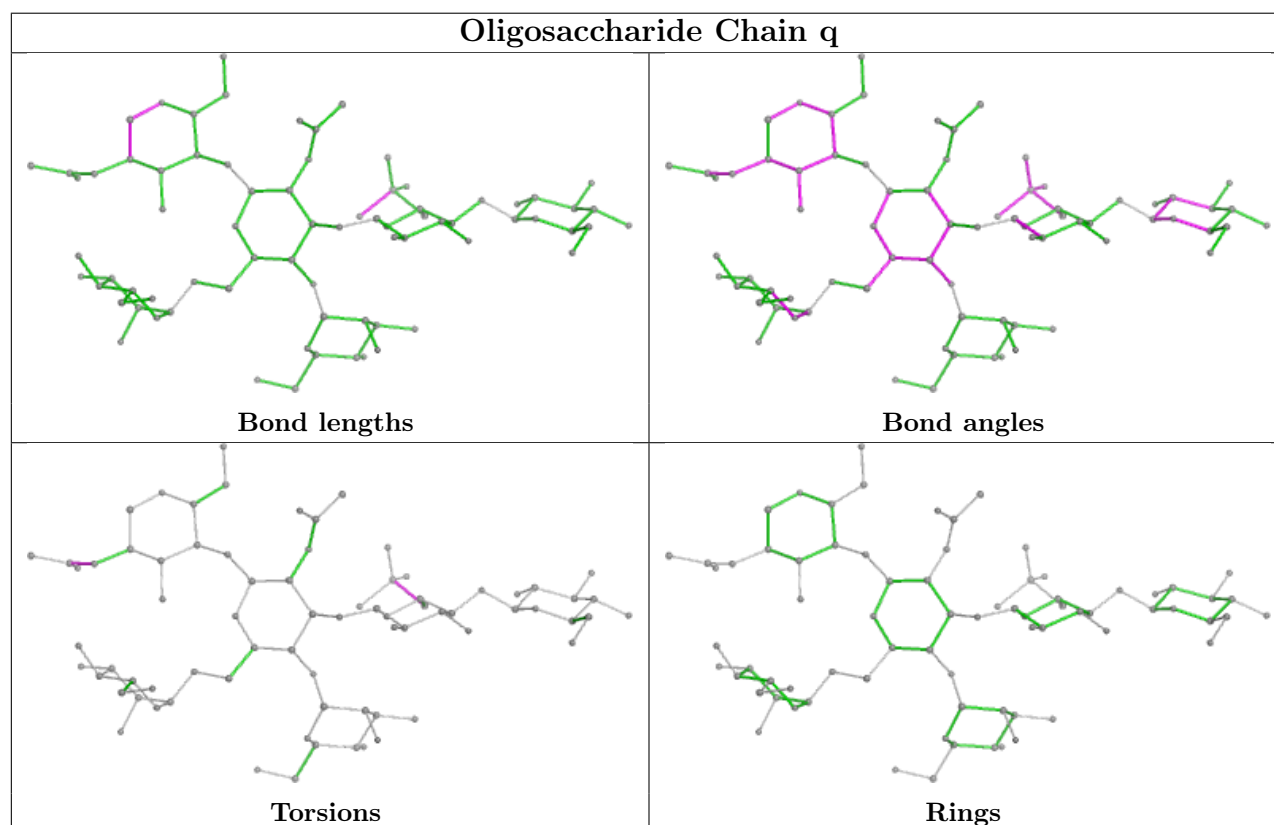
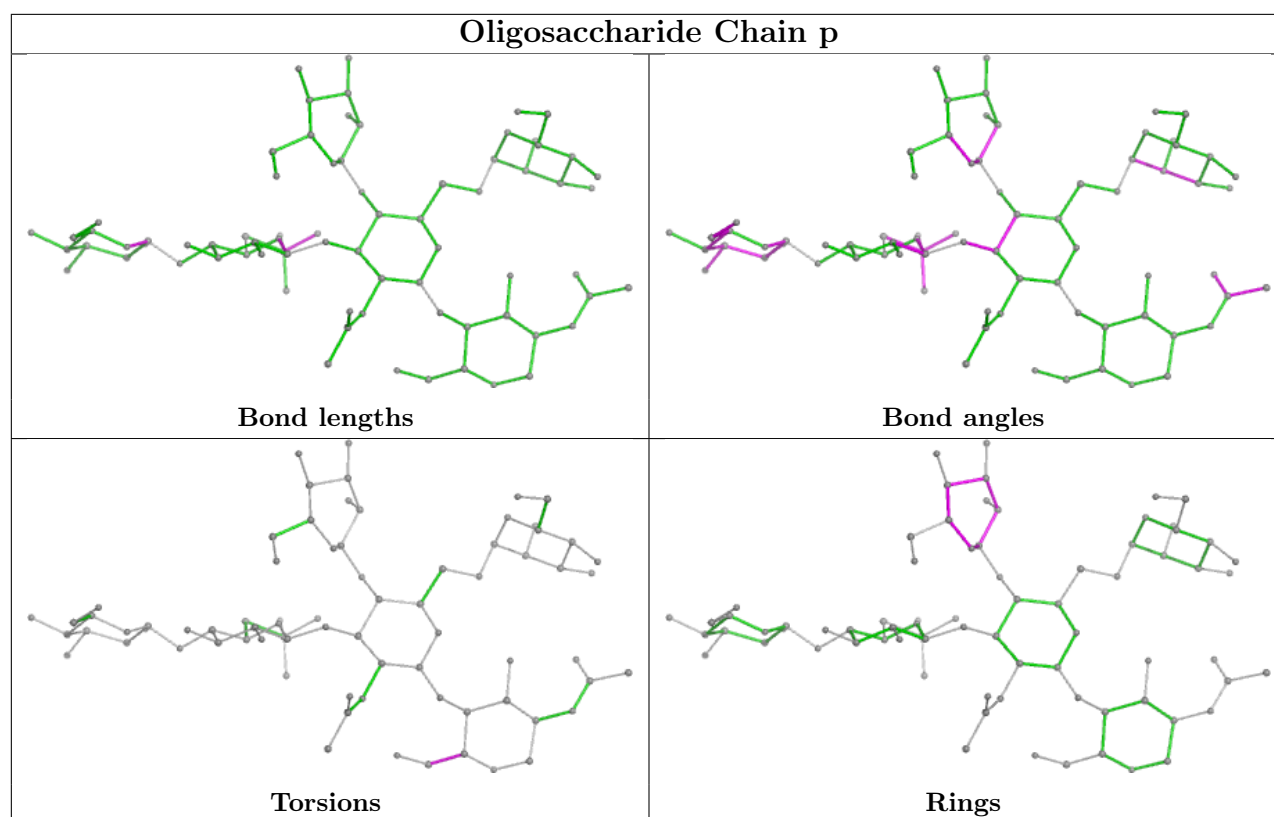


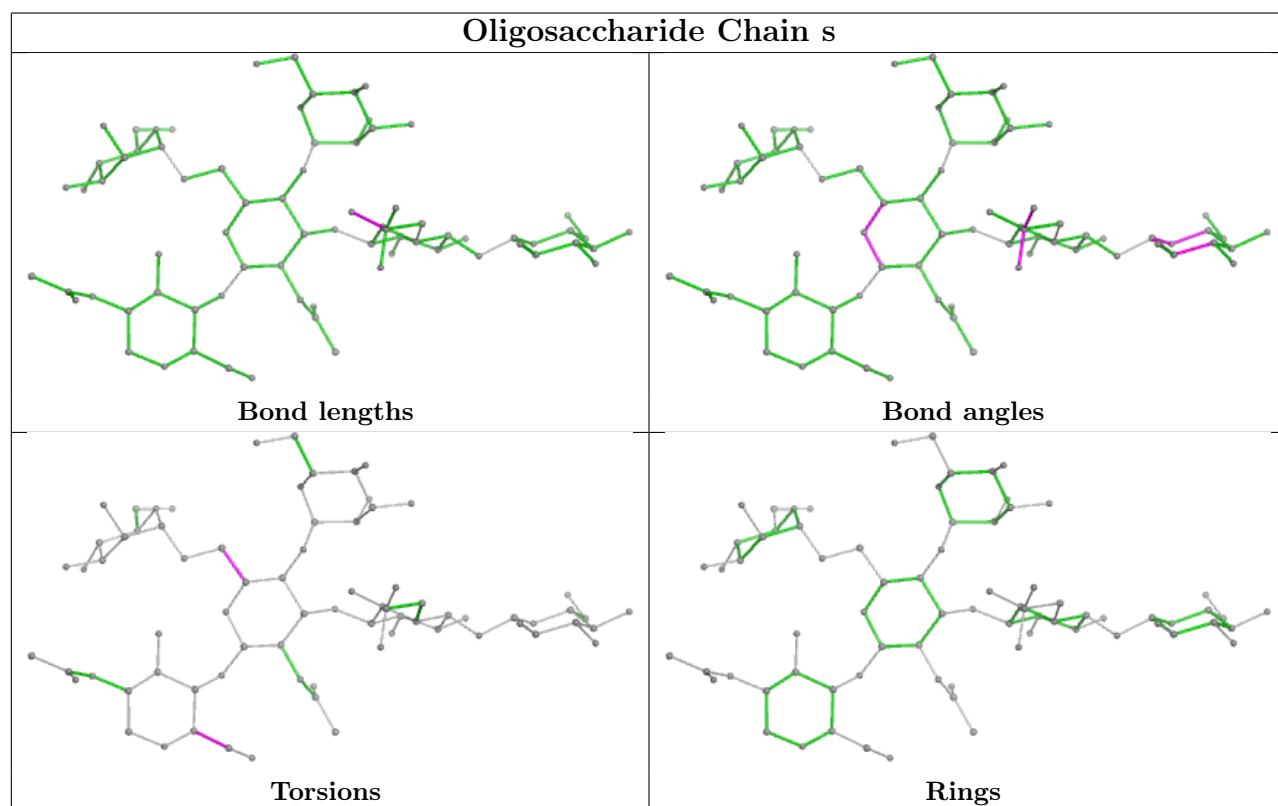
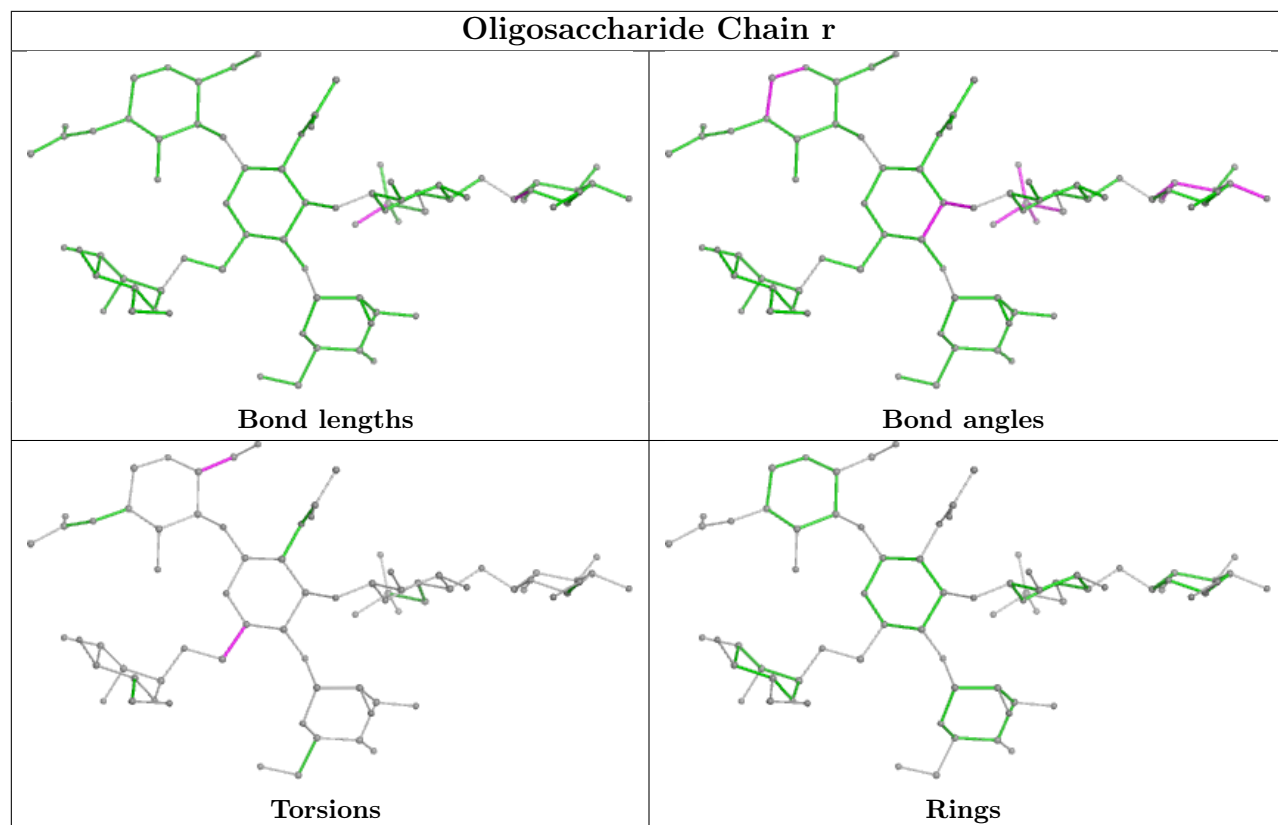


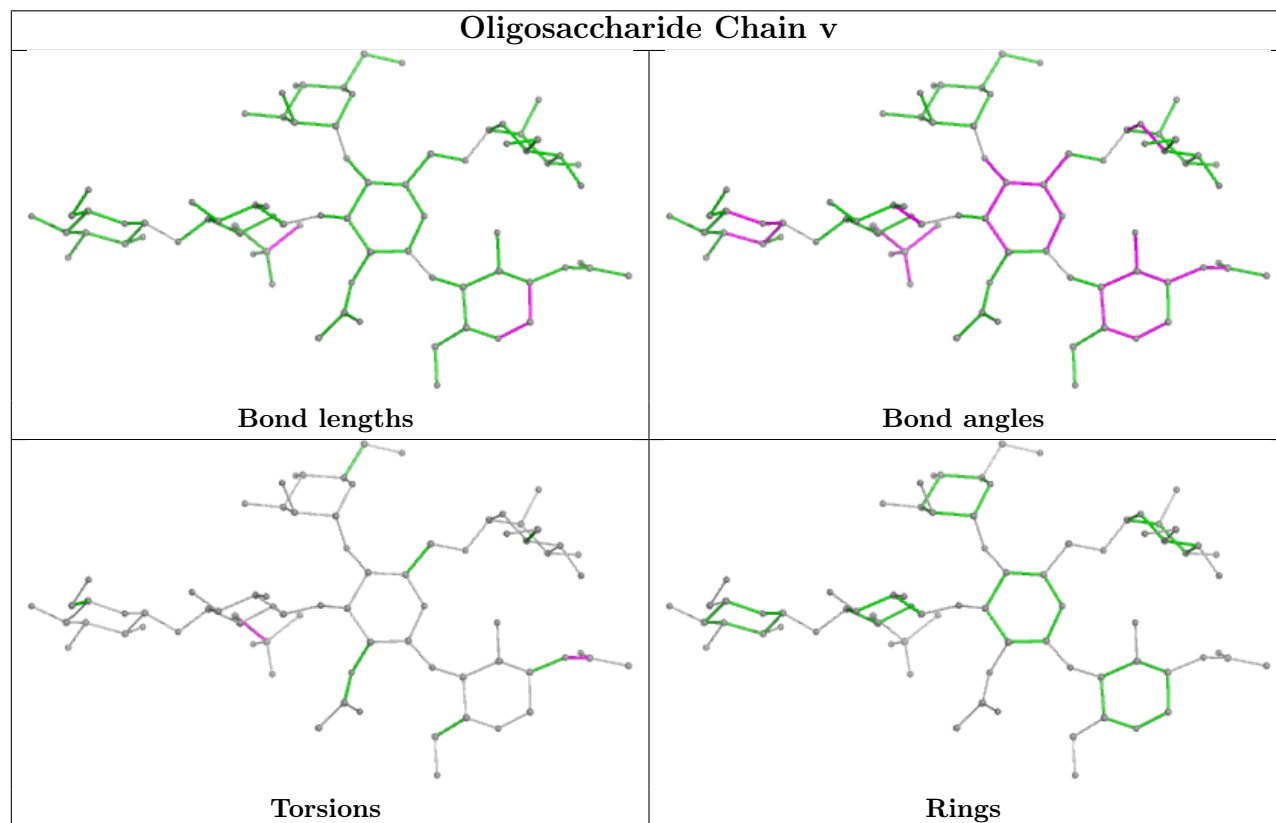
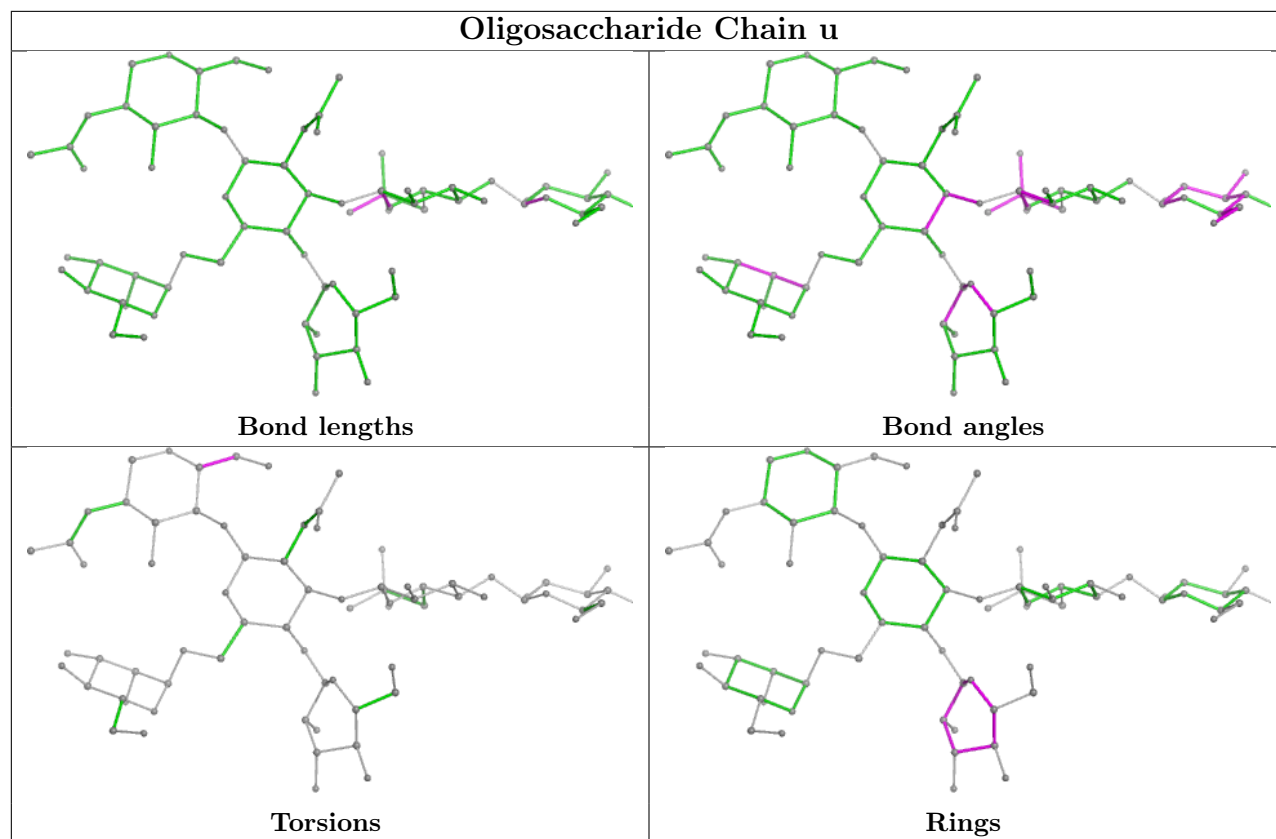


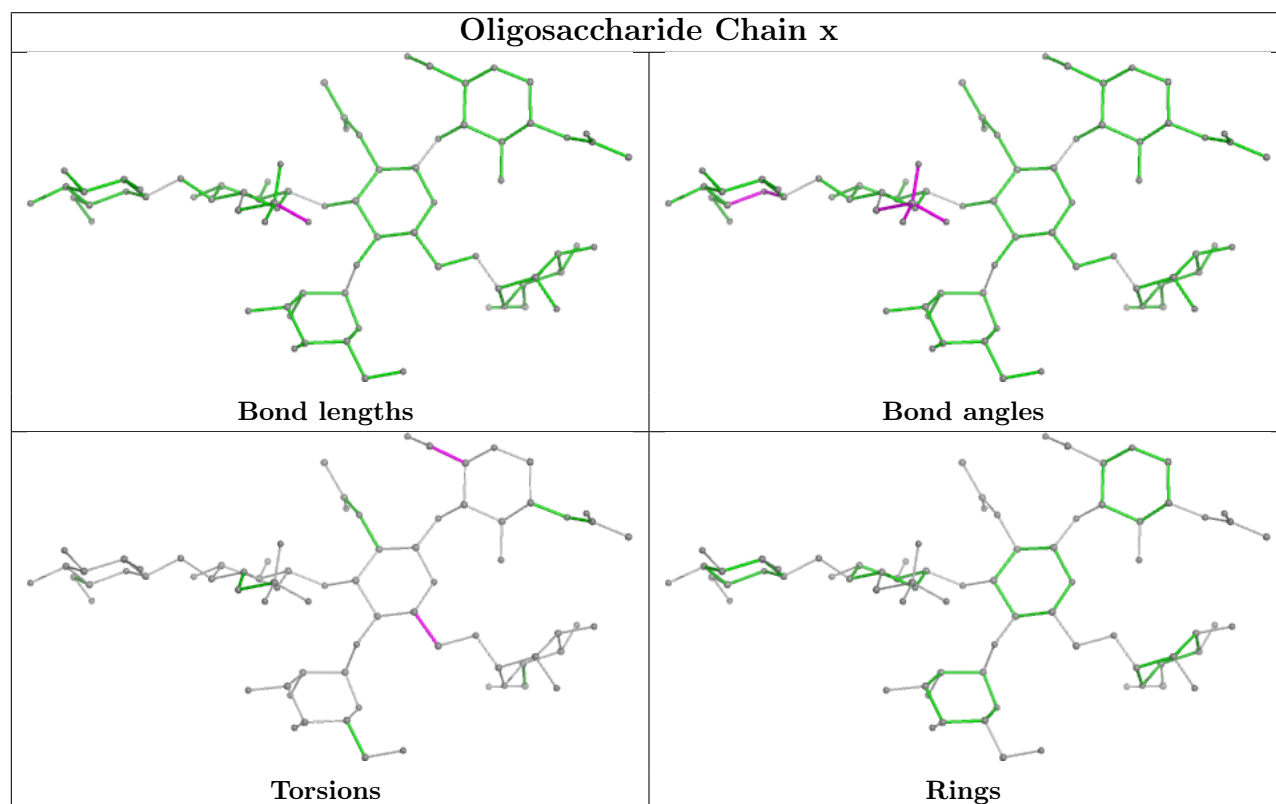
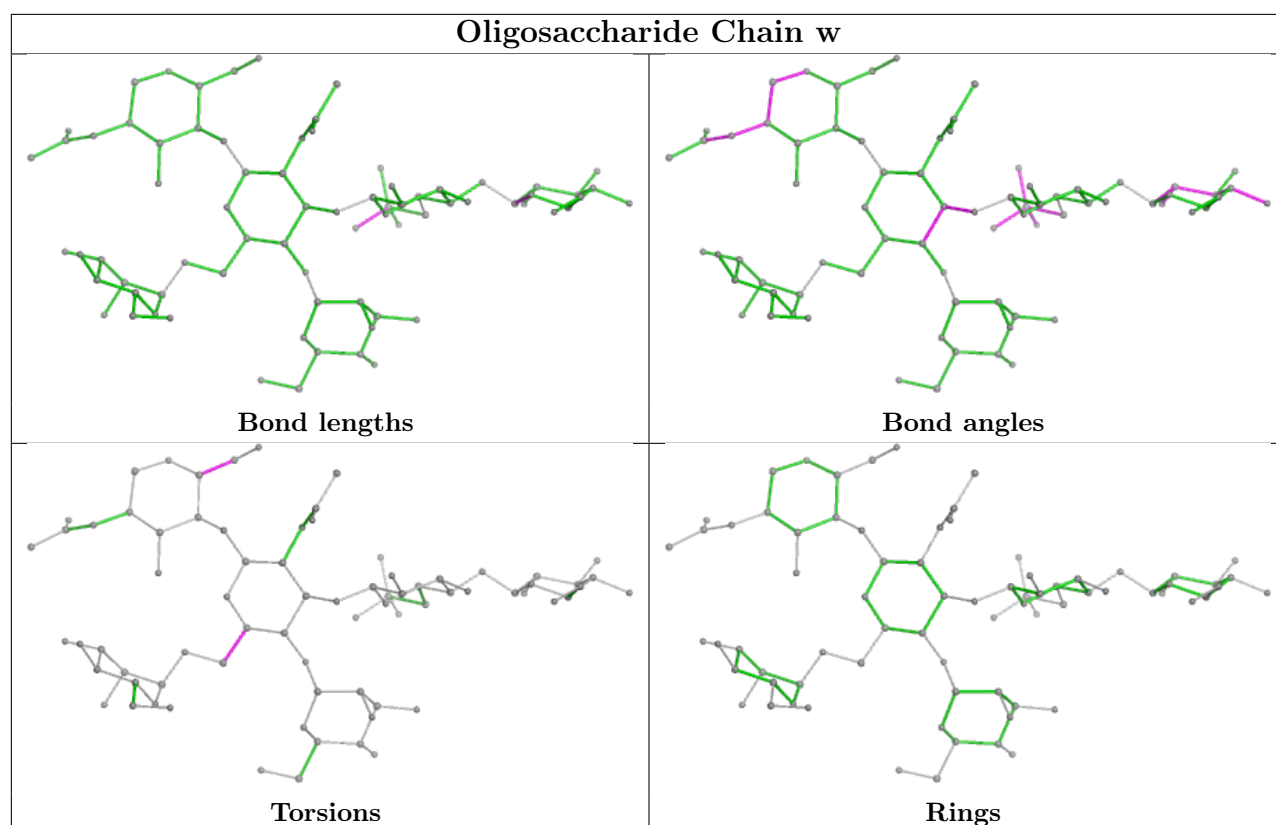


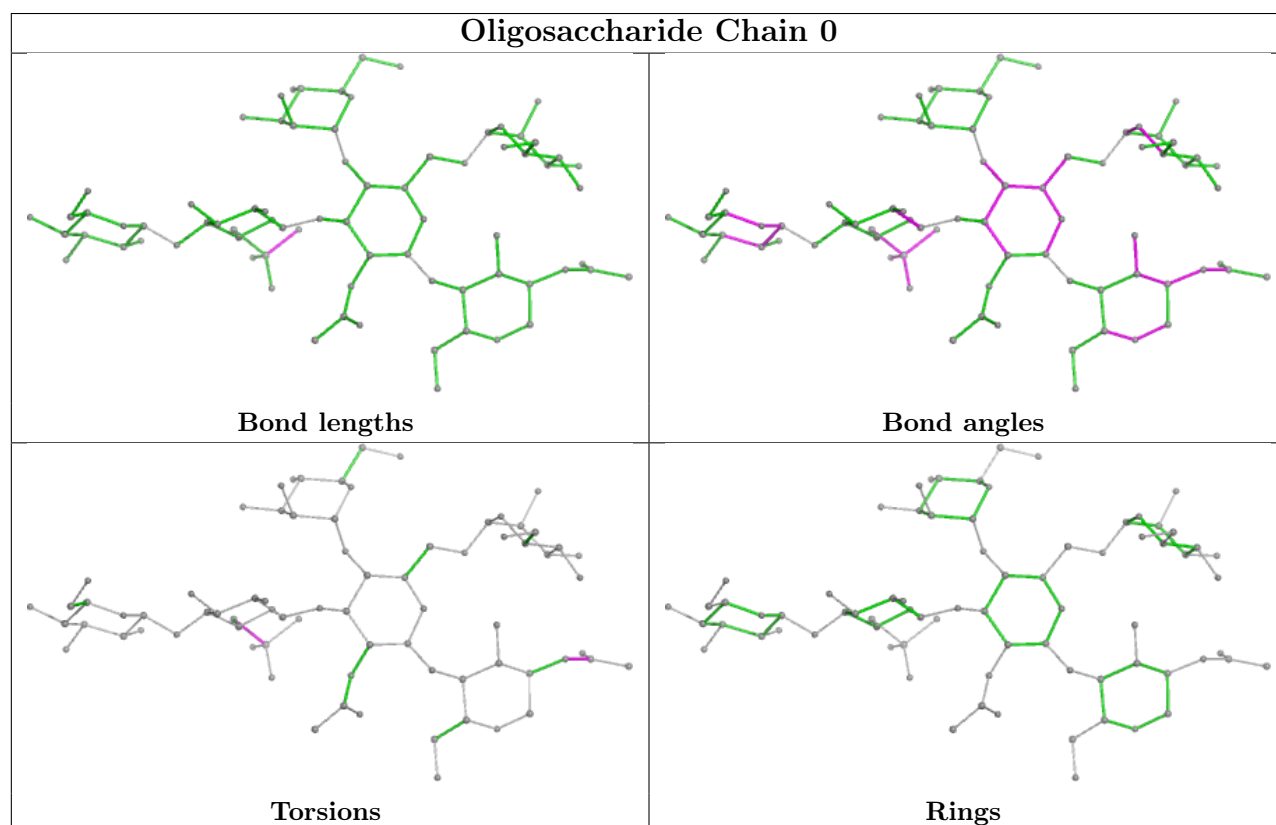
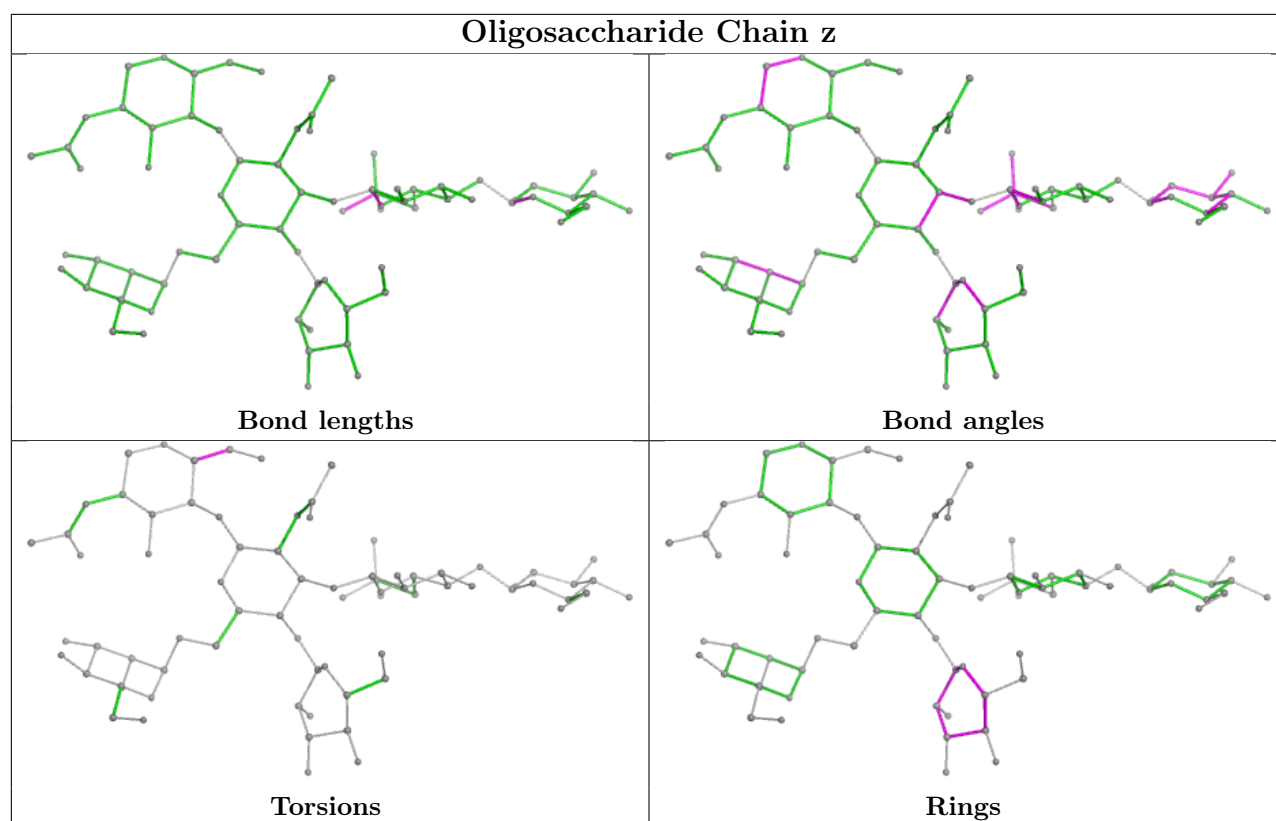


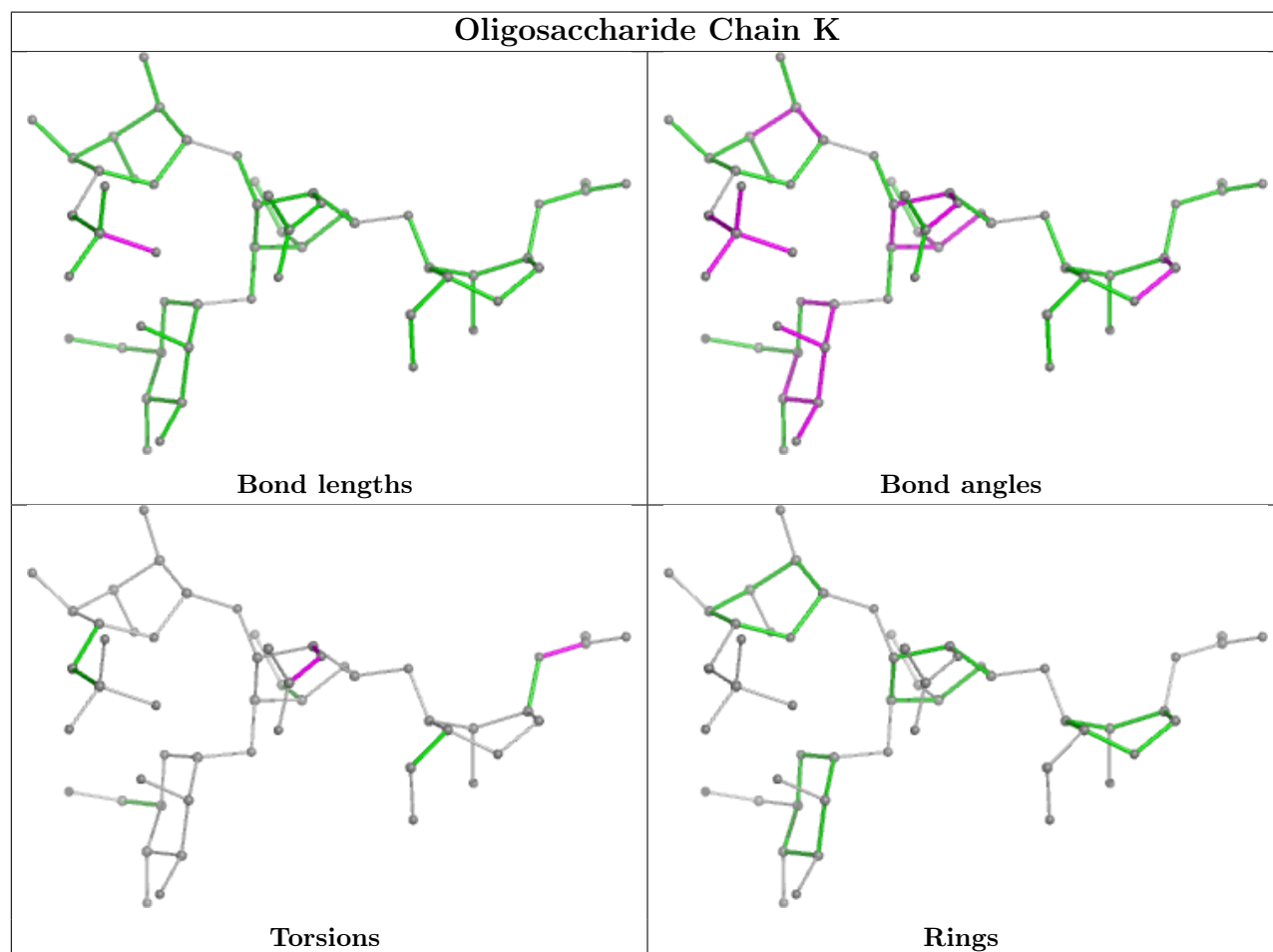
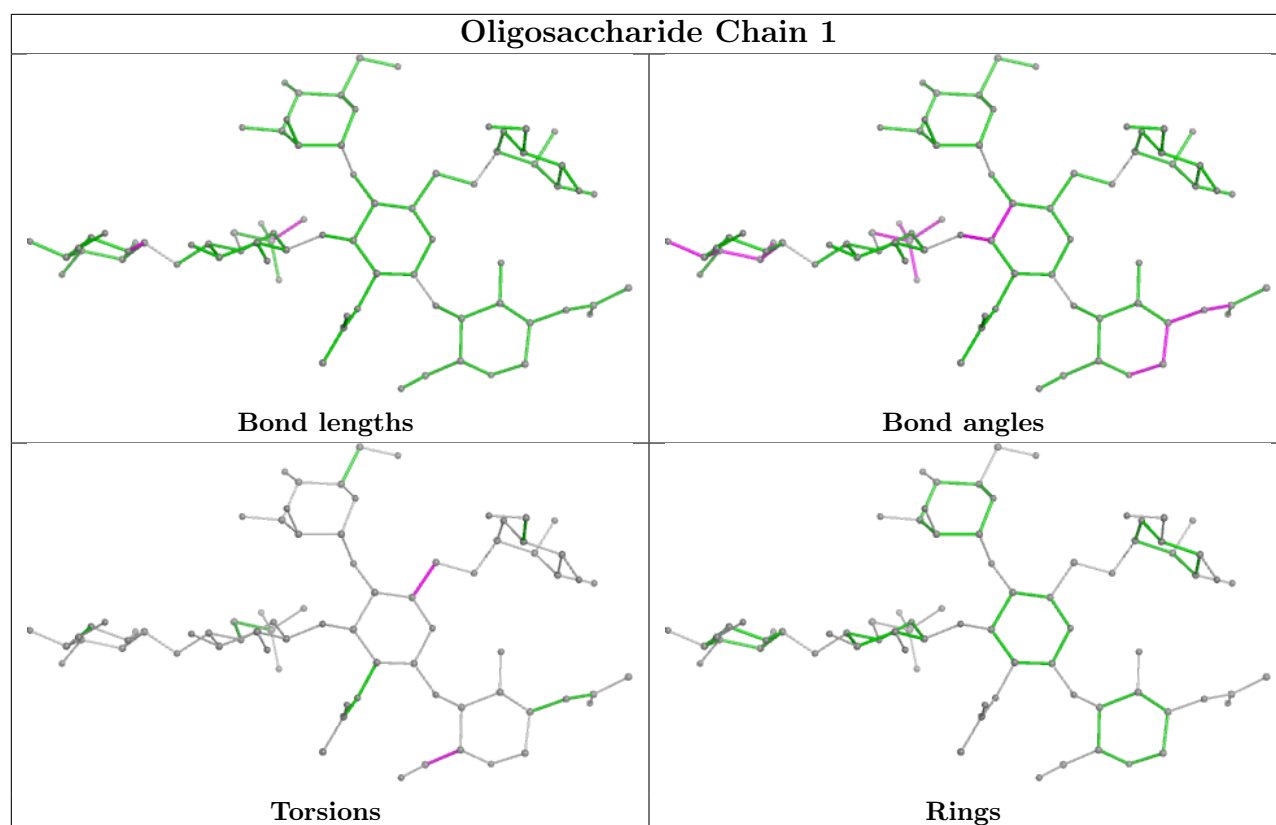


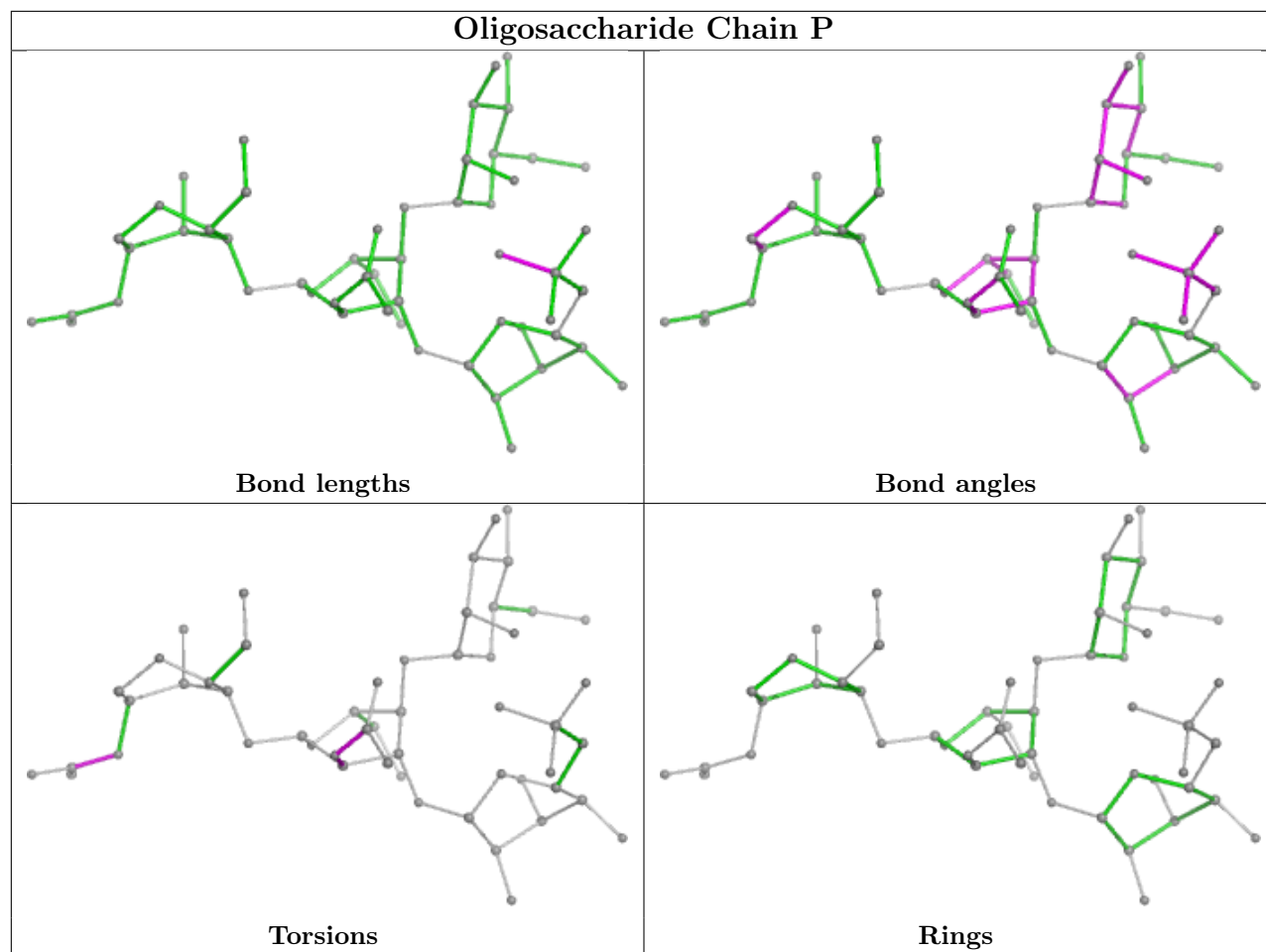


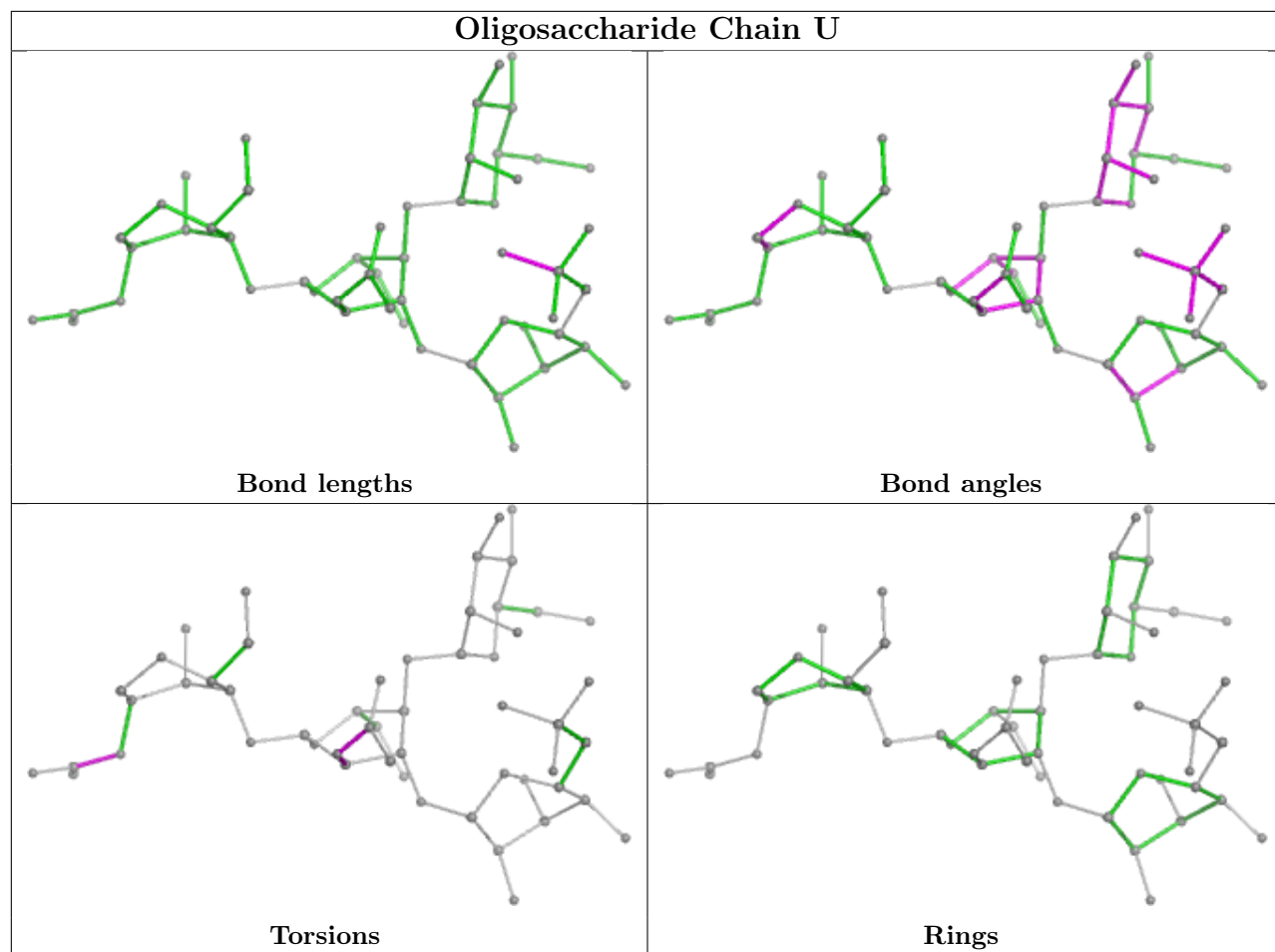


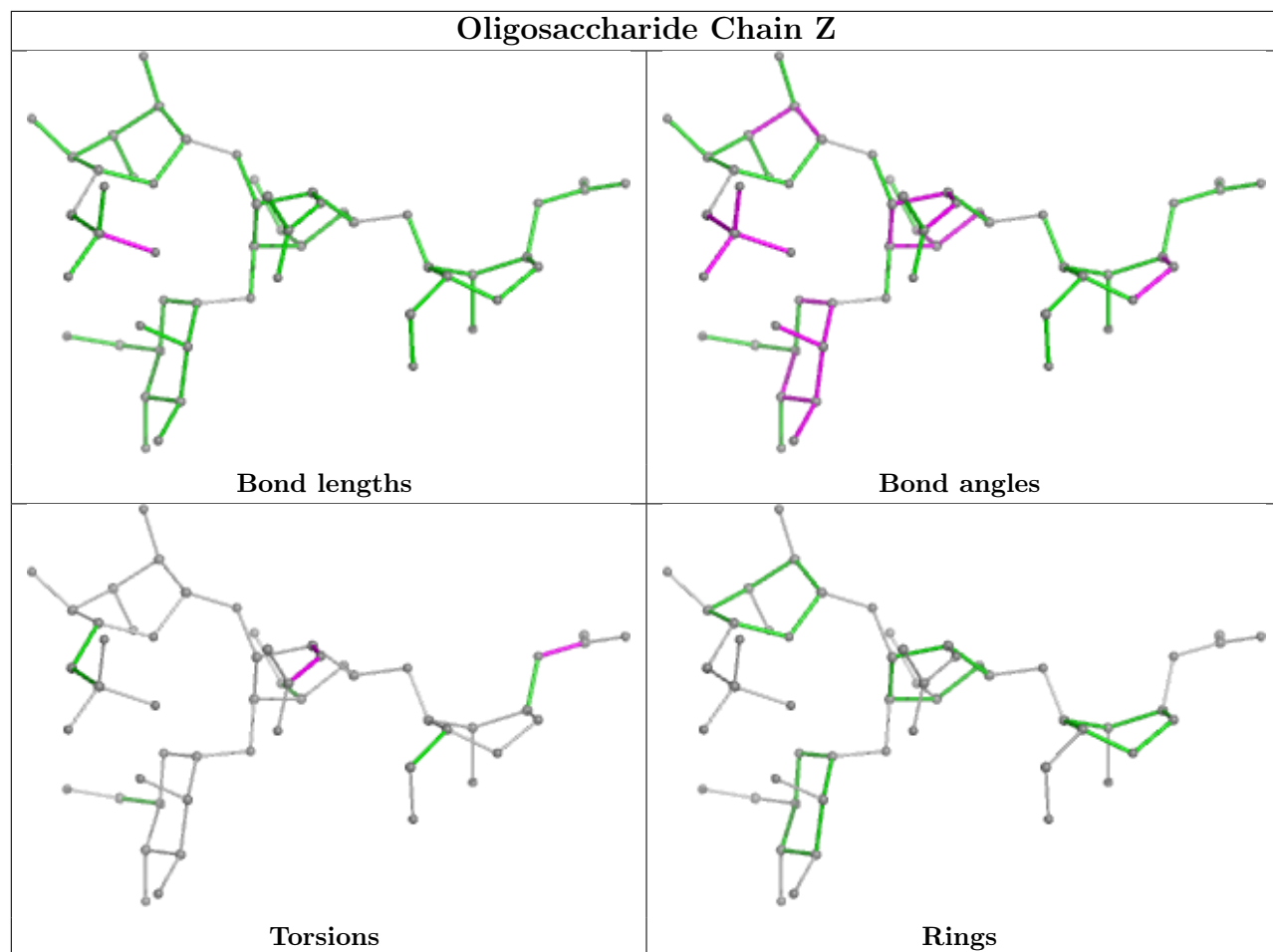


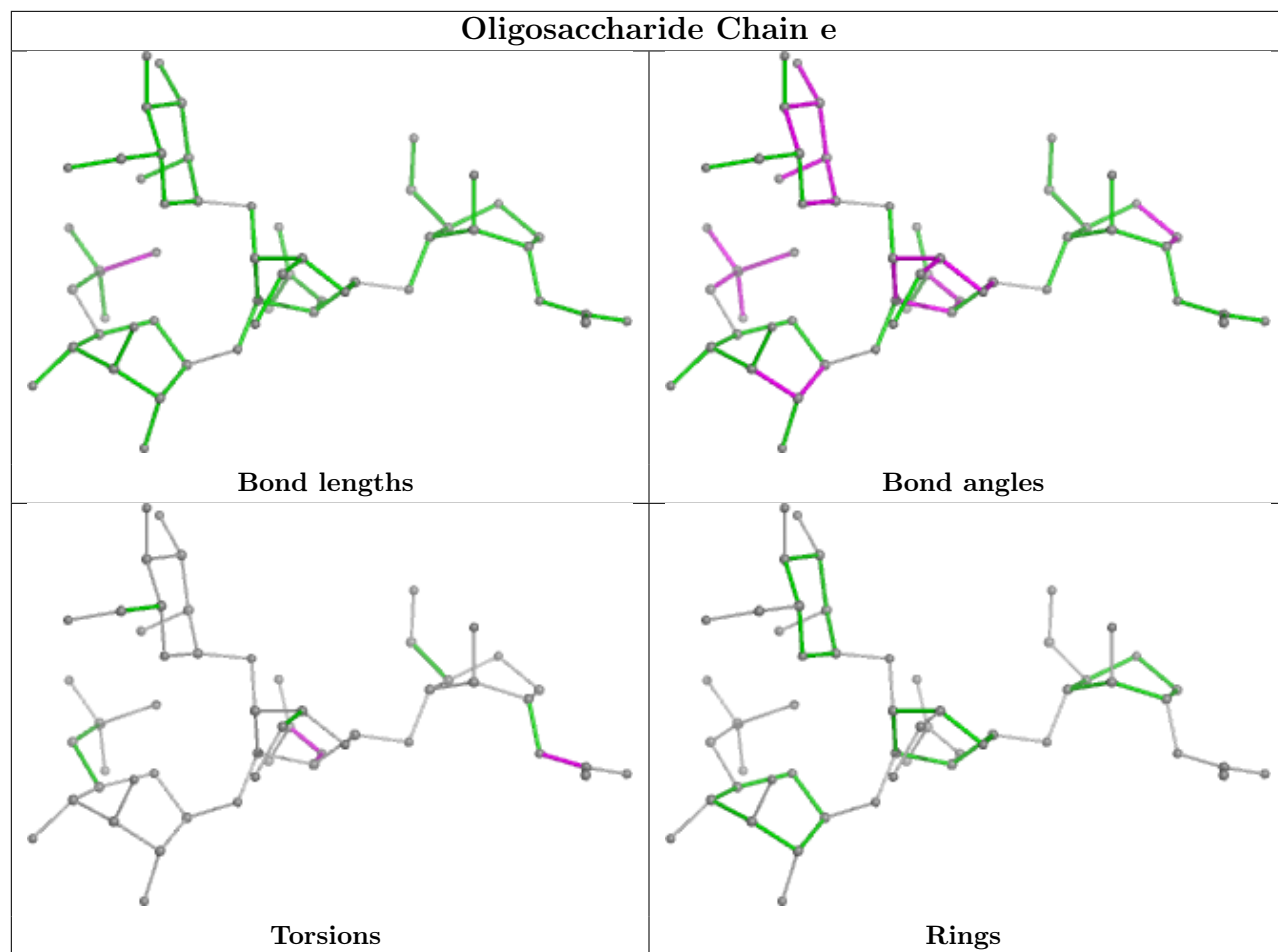


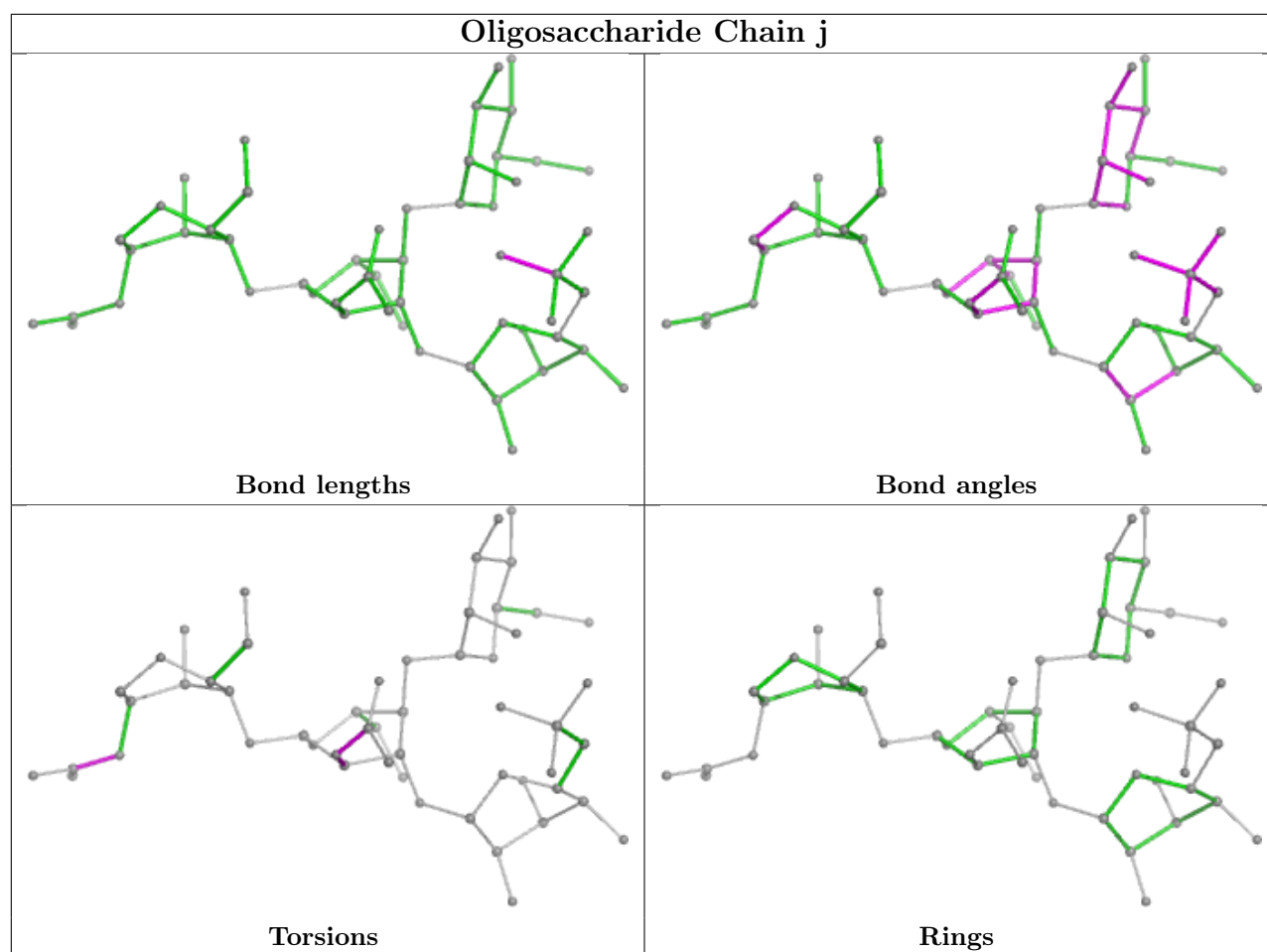


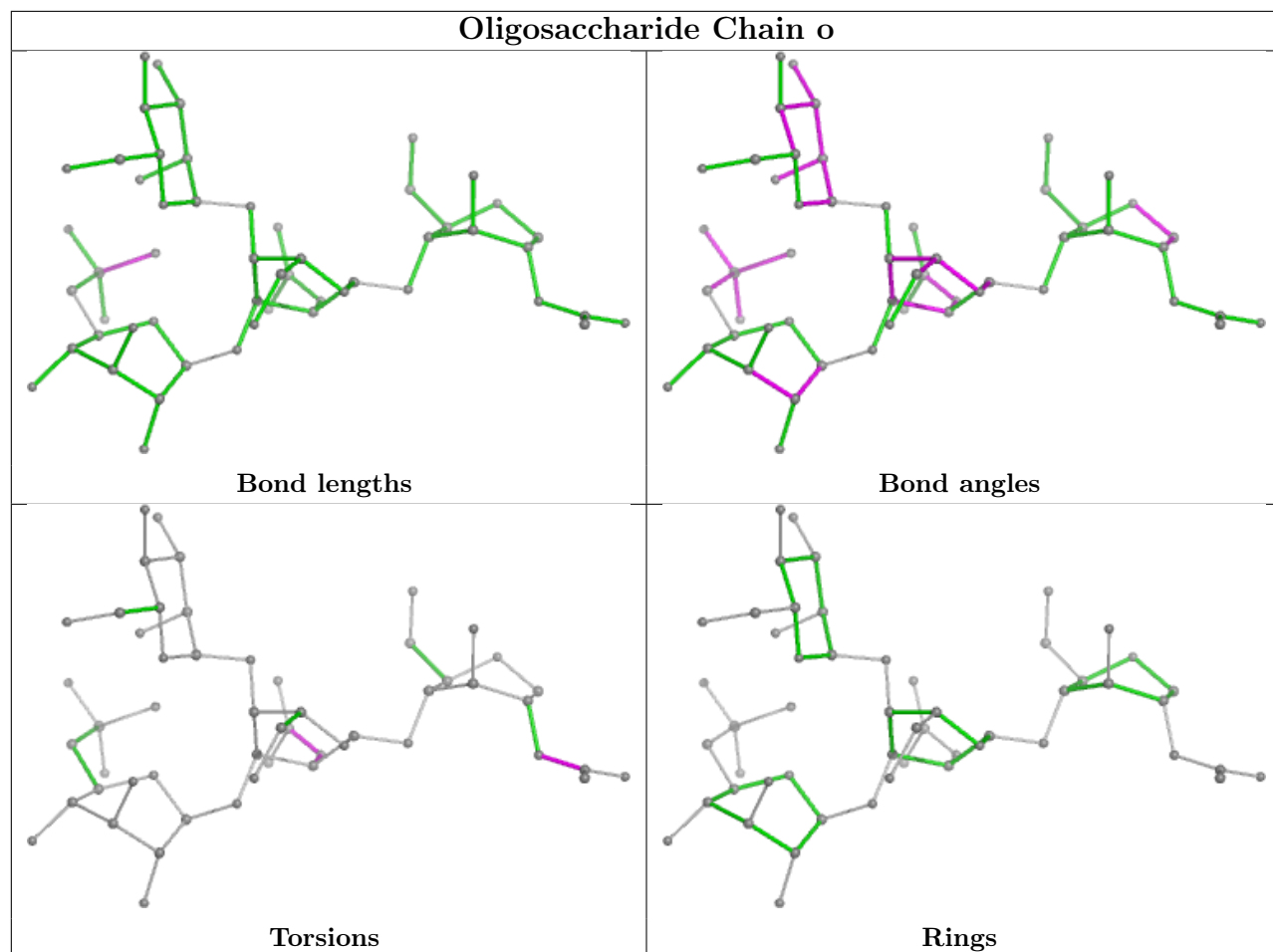


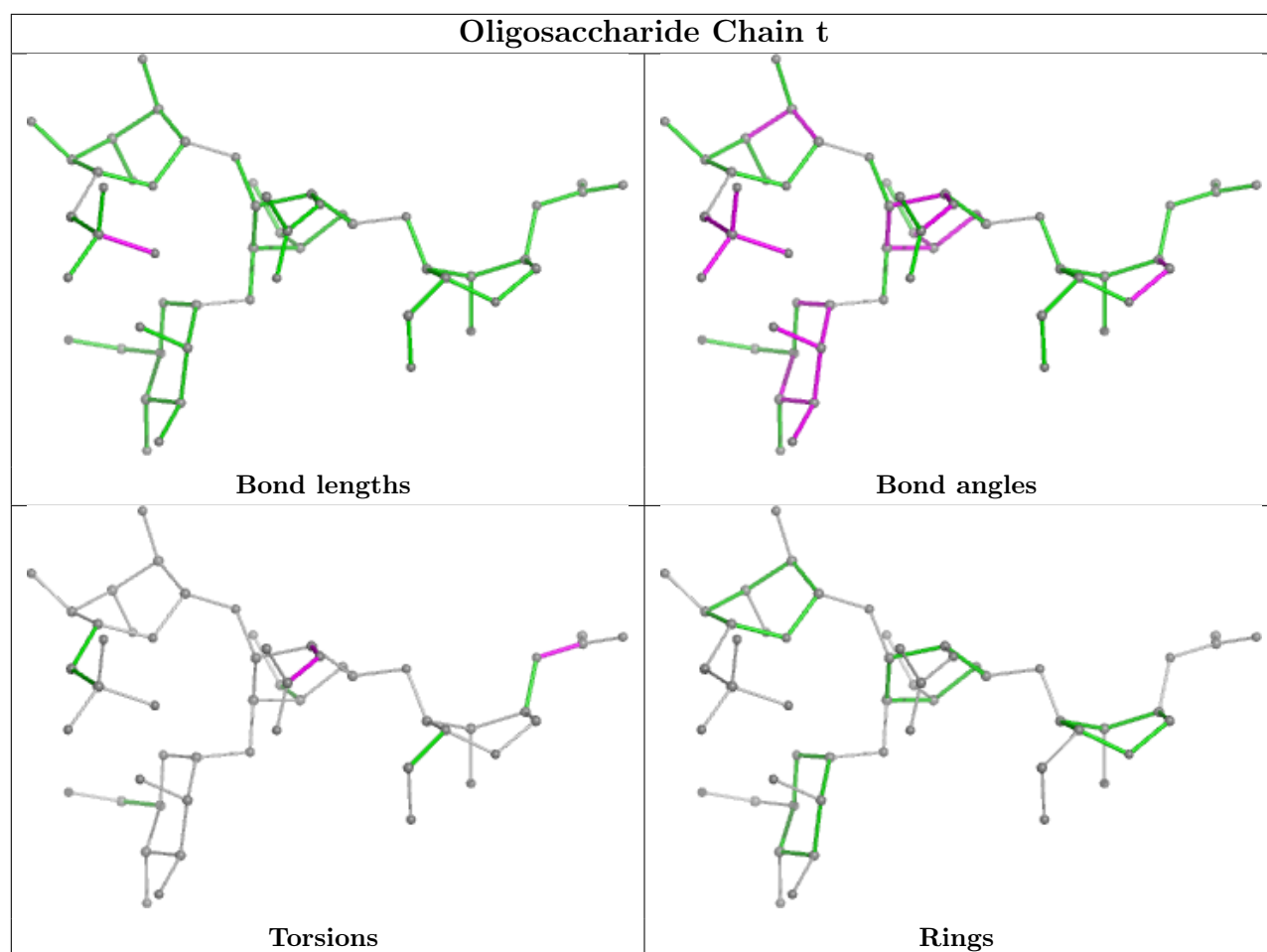


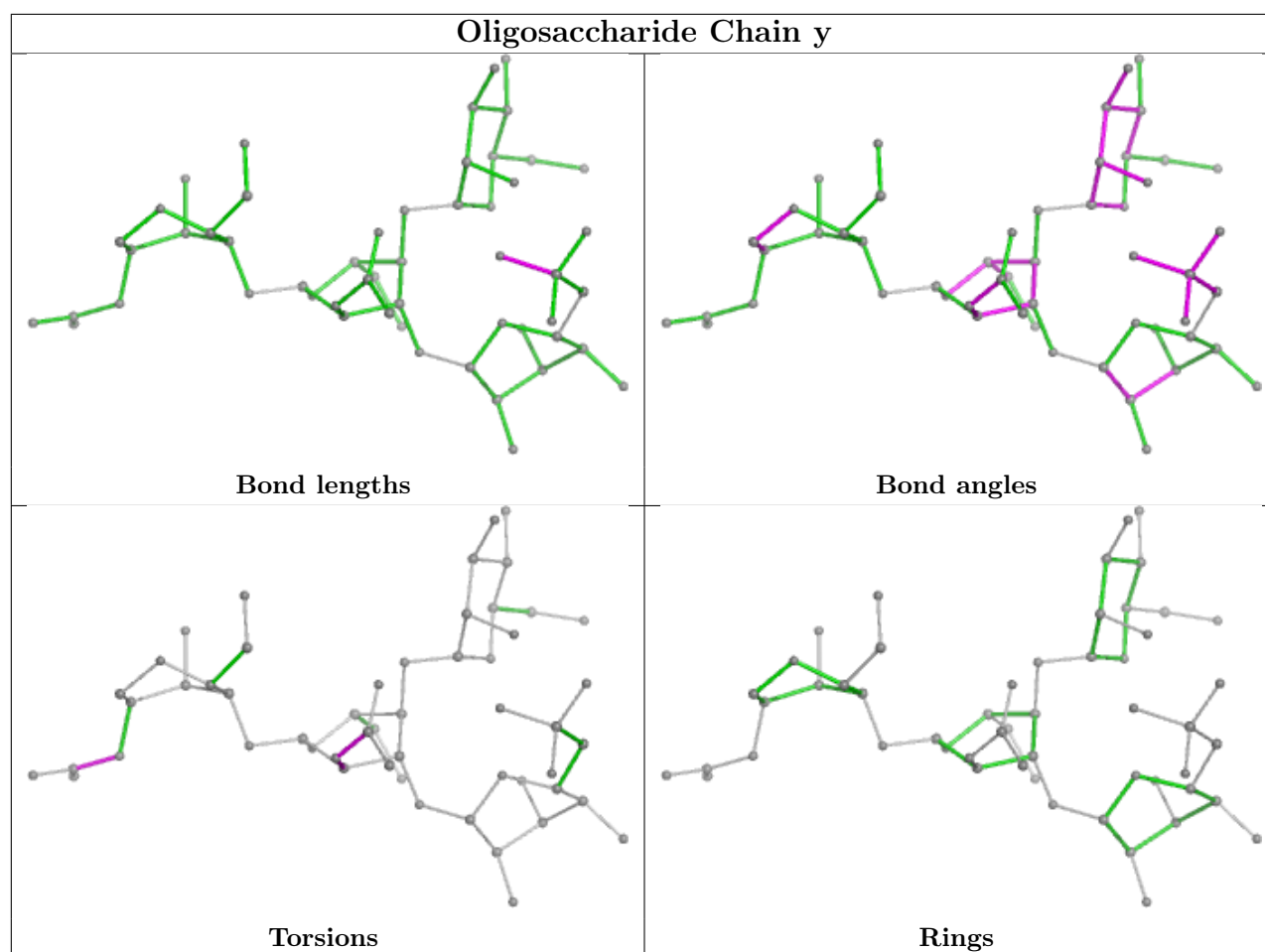












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

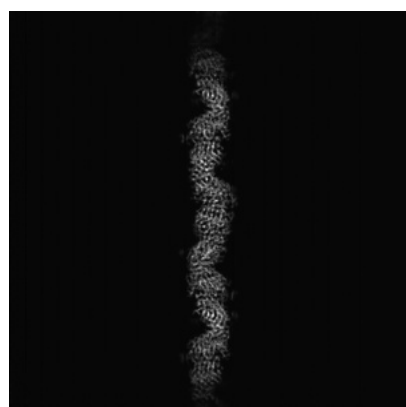
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13546. These allow visual inspection of the internal detail of the map and identification of artifacts.

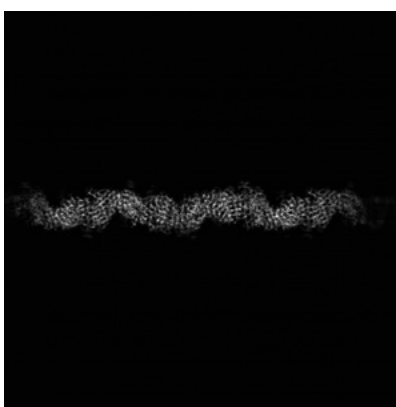
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

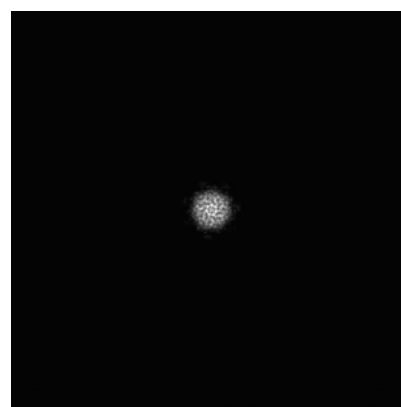
6.1.1 Primary map



X



Y



Z

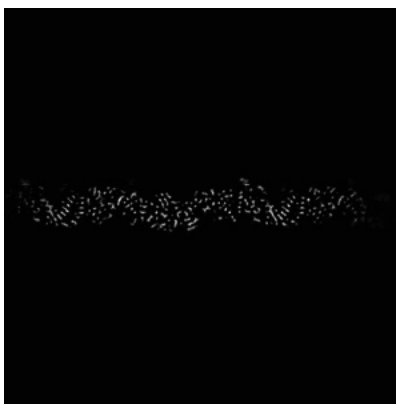
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

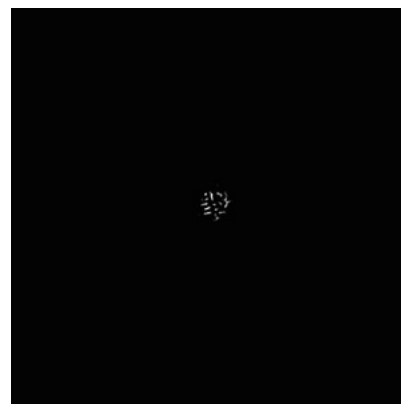
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 196



Y Index: 195

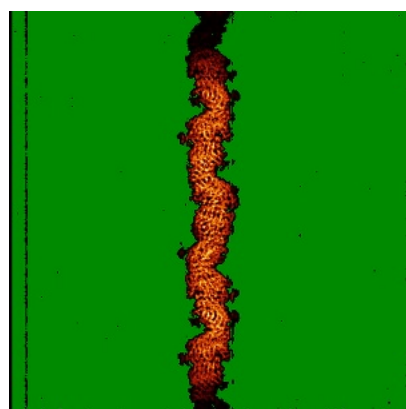


Z Index: 212

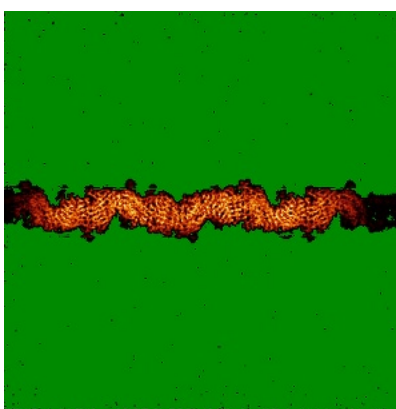
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

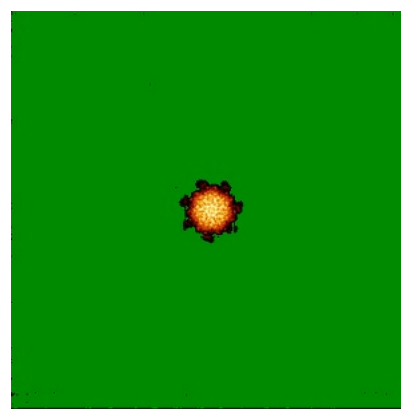
6.4.1 Primary map



X



Y

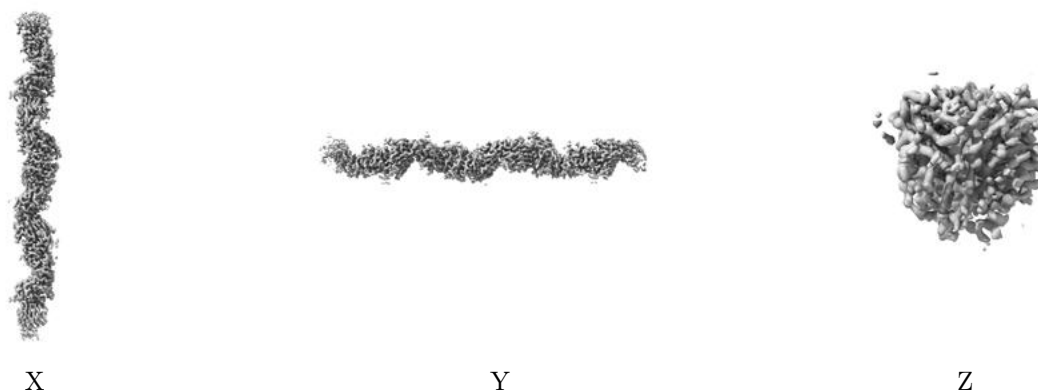


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1638. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

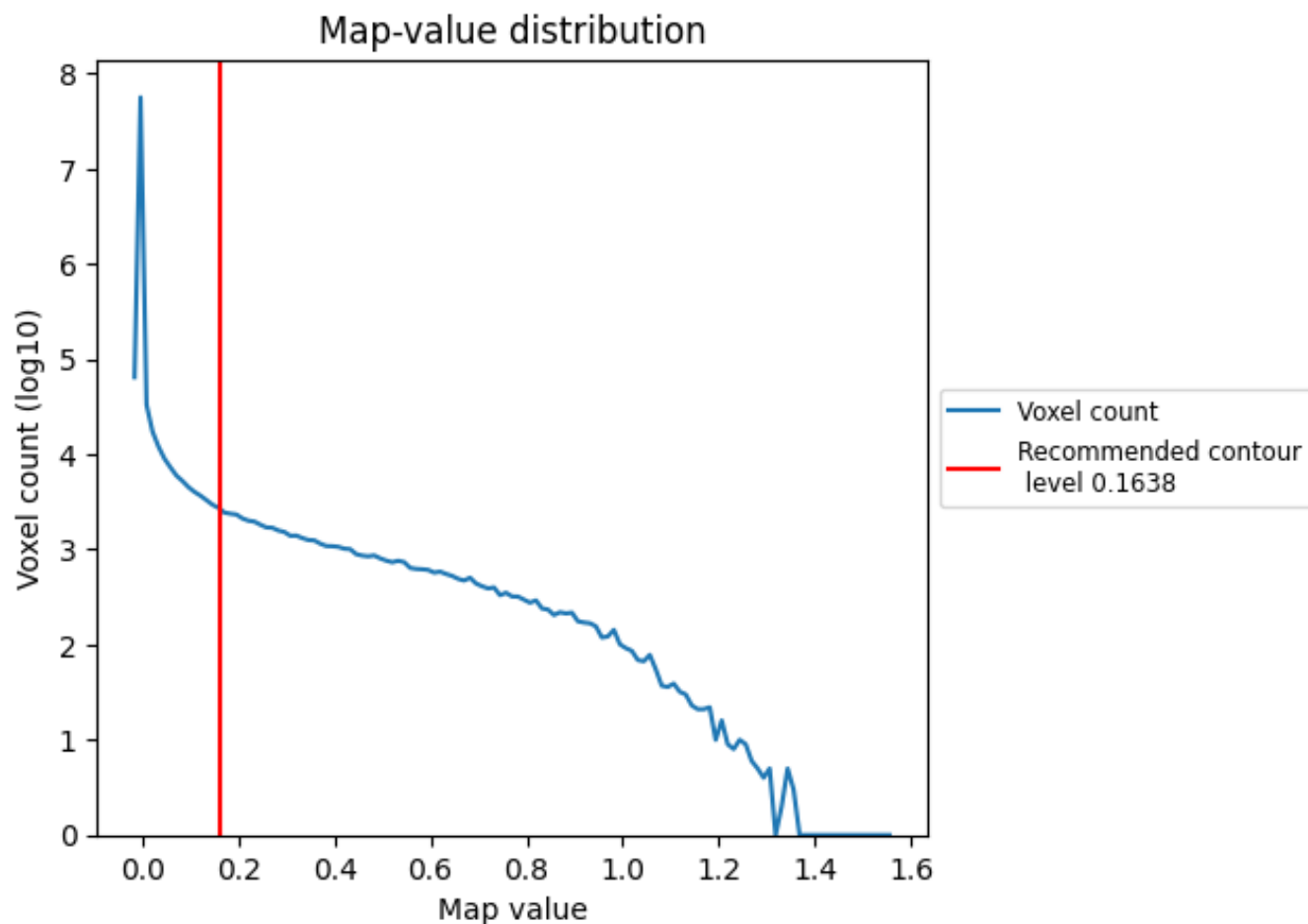
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

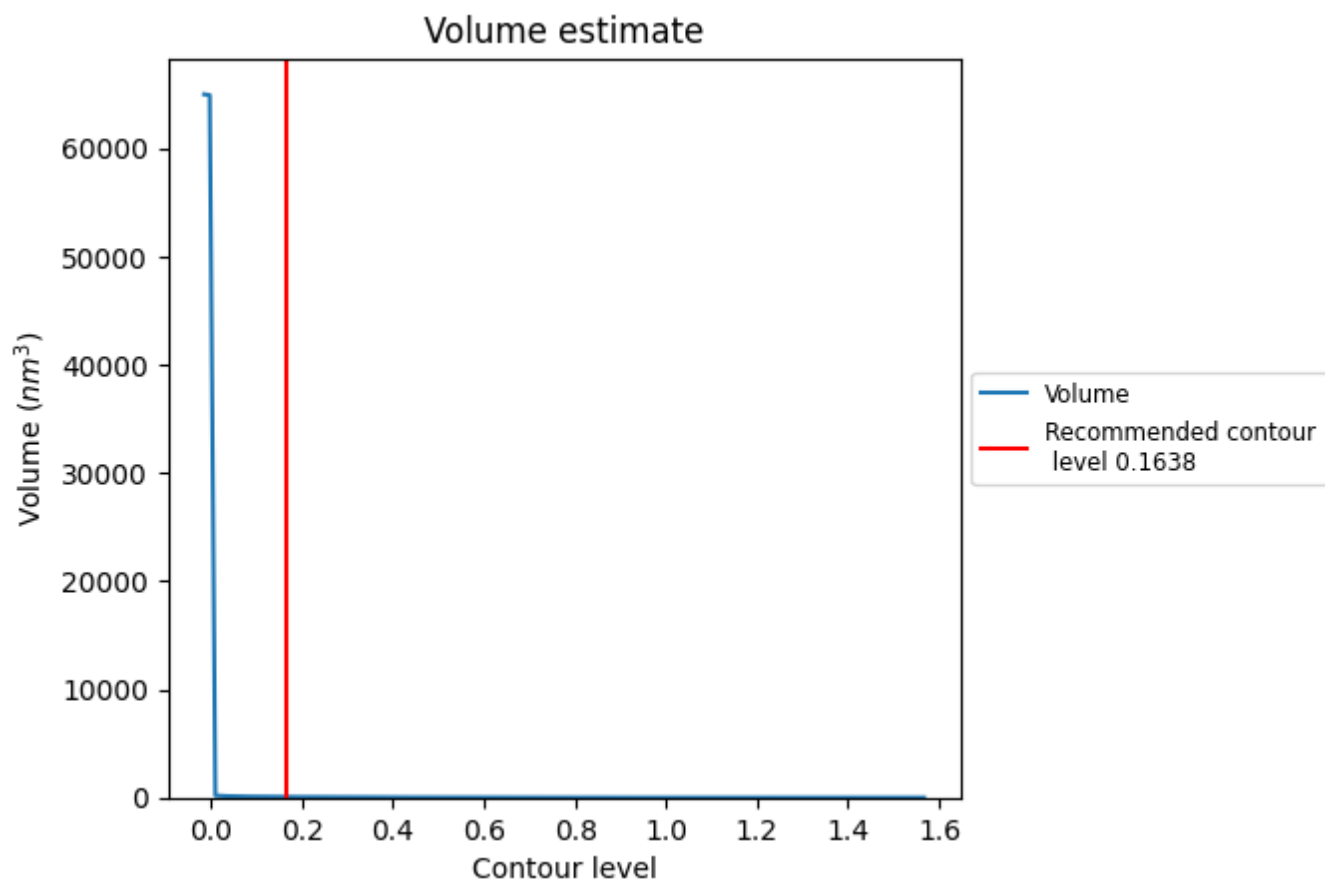
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

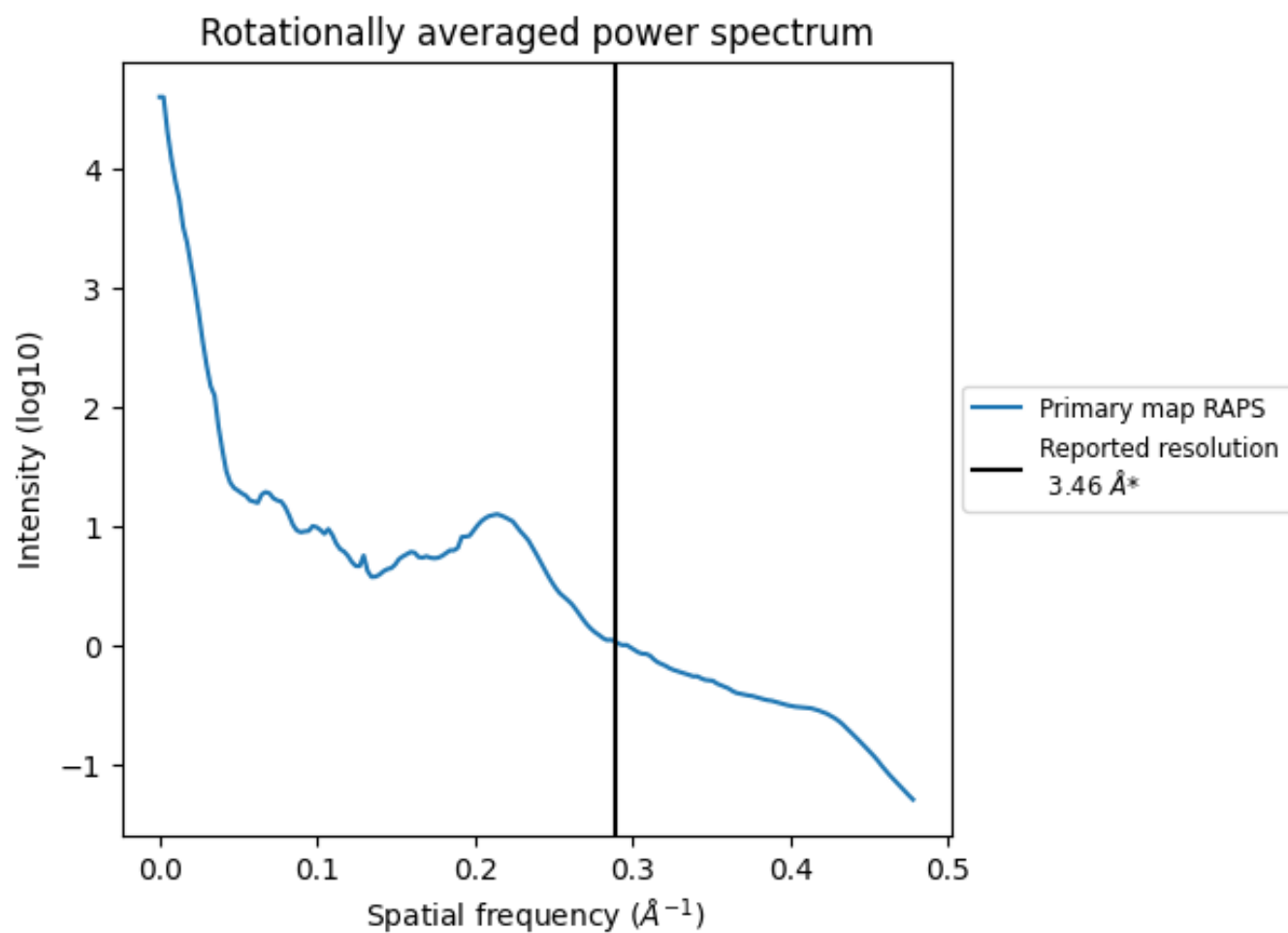
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm³; this corresponds to an approximate mass of 59 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

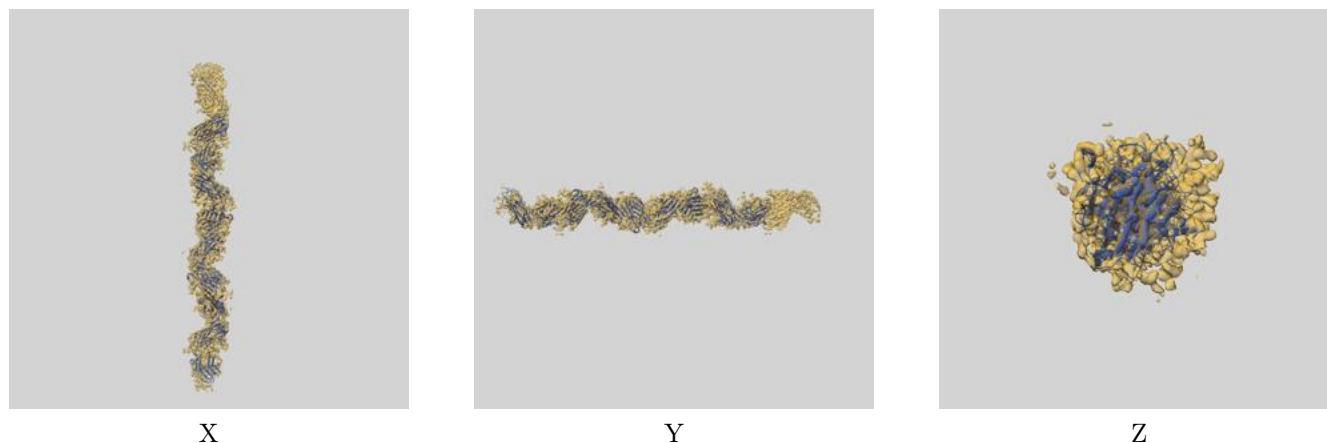
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

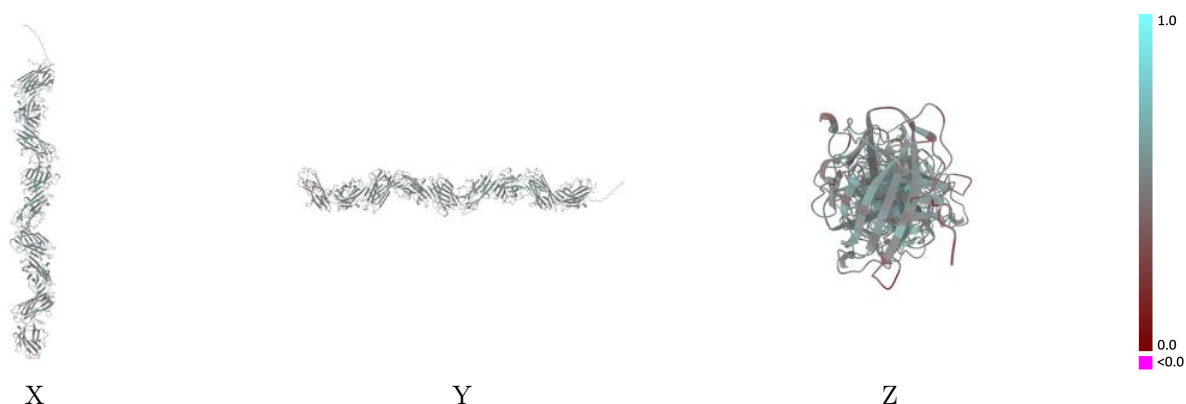
This section contains information regarding the fit between EMDB map EMD-13546 and PDB model 7PNB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



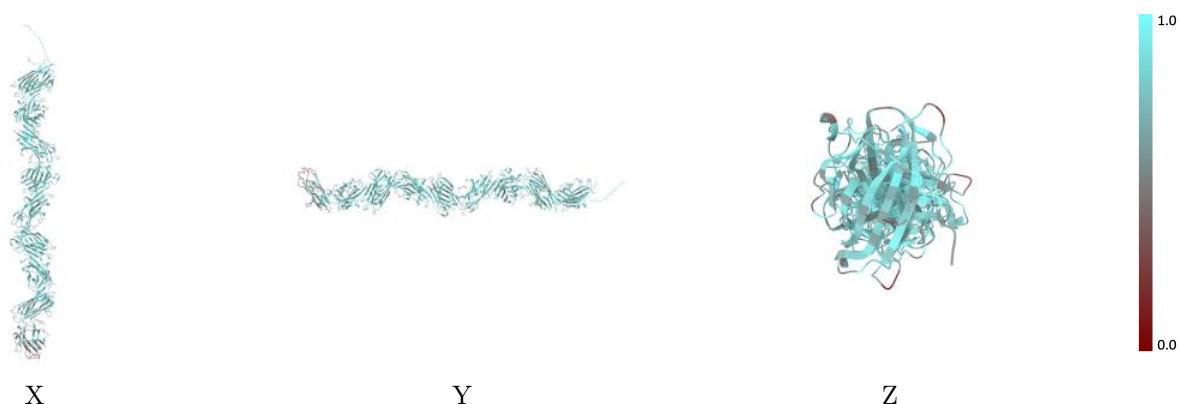
The images above show the 3D surface view of the map at the recommended contour level 0.1638 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



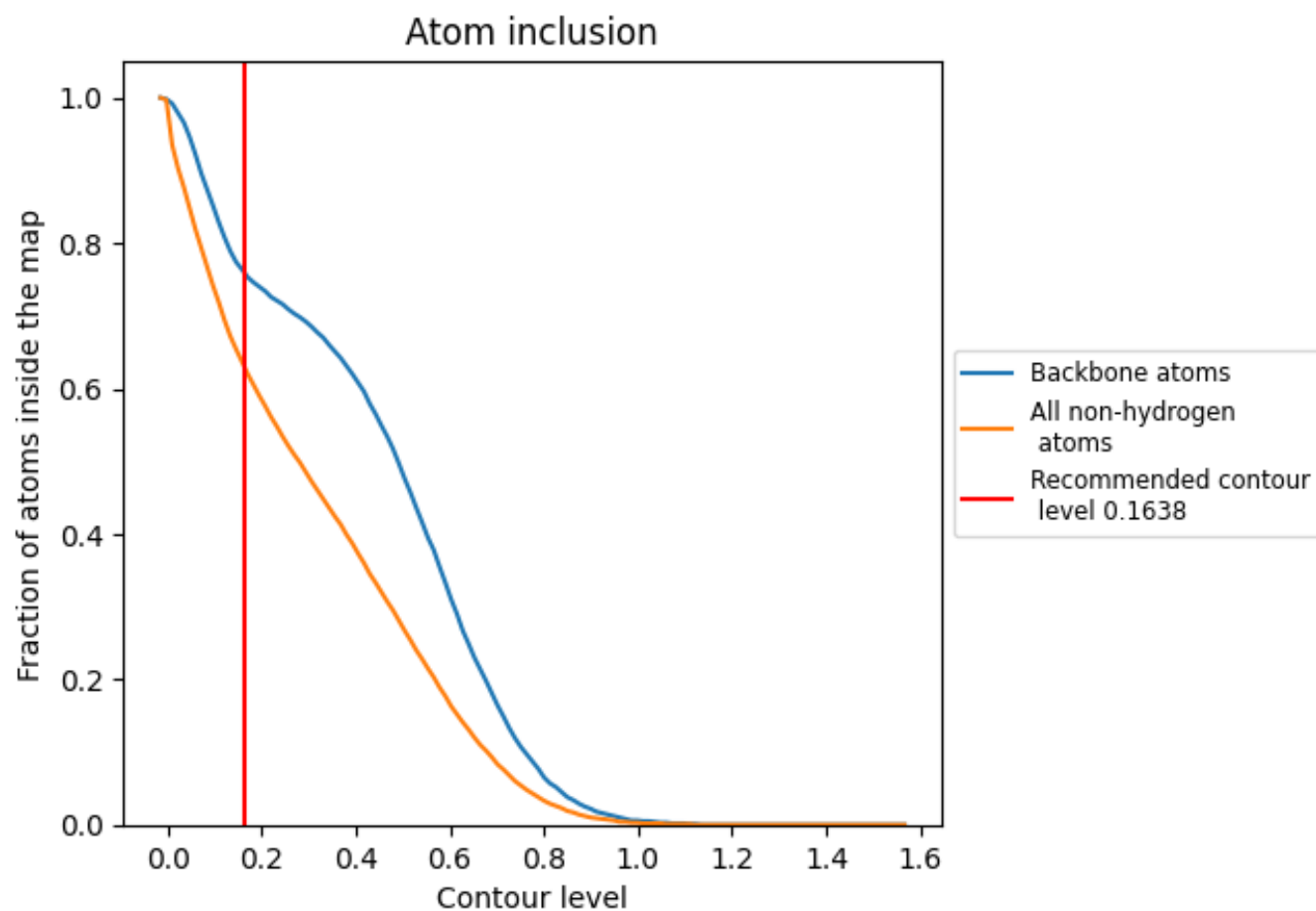
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1638).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.1638) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6290	 0.4610
0	 0.2130	 0.2910
1	 0.0270	 0.2120
A	 0.7060	 0.4830
B	 0.7180	 0.5040
C	 0.7330	 0.5140
D	 0.7320	 0.5170
E	 0.7240	 0.5110
F	 0.7270	 0.5080
G	 0.7220	 0.4920
H	 0.6960	 0.4810
I	 0.5440	 0.4440
J	 0.5870	 0.4630
K	 0.1130	 0.0520
L	 0.4800	 0.3380
M	 0.5730	 0.3920
N	 0.2270	 0.2480
O	 0.5600	 0.4350
P	 0.1510	 0.1150
Q	 0.5200	 0.4260
R	 0.5600	 0.4190
S	 0.1600	 0.2180
T	 0.5870	 0.4610
U	 0.1320	 0.1610
V	 0.5200	 0.4000
W	 0.5870	 0.4430
X	 0.1330	 0.2770
Y	 0.6130	 0.4740
Z	 0.1130	 0.2060
a	 0.4400	 0.3890
b	 0.6130	 0.4390
c	 0.2400	 0.3070
d	 0.6130	 0.4510
e	 0.1320	 0.1640
f	 0.3600	 0.4070



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Chain	Atom inclusion	Q-score
g	 0.5600	 0.4200
h	 0.2670	 0.2730
i	 0.6000	 0.4560
j	 0.1510	 0.2180
k	 0.4800	 0.3930
l	 0.5330	 0.4040
m	 0.1470	 0.2500
n	 0.5600	 0.4480
o	 0.1510	 0.1980
p	 0.3470	 0.3610
q	 0.5200	 0.4170
r	 0.0930	 0.2560
s	 0.4400	 0.3790
t	 0.1130	 0.0370
u	 0.2800	 0.3340
v	 0.4800	 0.3610
w	 0.1330	 0.2660
x	 0.0670	 0.2750
y	 0.0380	 0.0170
z	 0.0670	 0.2630